

Support Vector Regression

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Advanced Machine Learning

Sparse Solution

- SVM classification is a sparse algorithm. The final solution consists of a subset of training points called support vectors support vectors.
- Such a representation has computational advantageous
- SVM regression use ϵ insensitive loss function to ensure sparseness of the solution

Error Tolerance: ϵ

- No error
 - $|y - \tilde{f}(x)| \leq \epsilon$
 - $-\epsilon \leq y - \tilde{f}(x) \leq \epsilon$
- Error
 - $|y - \tilde{f}(x)| > \epsilon$
 - $y - \tilde{f}(x) < -\epsilon$ or $y - \tilde{f}(x) > \epsilon$

ϵ insensitive loss function

$$L^\epsilon(x, y, \tilde{f}) = |y - \tilde{f}(x)|_\epsilon = \max(0, |y - \tilde{f}(x)| - \epsilon)$$

- $\max(0, (y - \tilde{f}(x) - \epsilon)) = \xi$, $\max(0, (\tilde{f}(x) - y) - \epsilon) = \xi^*$
- ξ and ξ^* cannot be greater than zero at the same time.

Data

$$\{(x_1, y_1), (x_2, y_2) \dots (x_N, y_N)\}, x_i \in \mathbb{R}^n, y_i \in \mathbb{R}$$

$$\min_{f \in \mathcal{F}, b \in \mathbb{R}} \|f\|^2 + C \sum_{i=1}^N (\xi_i + \xi_i^*)$$

subject to

$$(y_i - \tilde{f}(x_i)) - \epsilon \leq \xi_i, \quad i = 1, \dots, N$$

$$(\tilde{f}(x_i) - y_i) - \epsilon \leq \xi_i^*, \quad i = 1, \dots, N$$

$$\xi_i \geq 0, \quad i = 1, \dots, N$$

$$\xi_i^* \geq 0, \quad i = 1, \dots, N$$

Case 1: Linear

- $\tilde{f}(x) = \langle w, x \rangle + b, w \in \mathbb{R}^n, b \in \mathbb{R}$

$$\min_{w \in \mathbb{R}^n, b \in \mathbb{R}} \|w\|^2 + C \sum_{i=1}^N (\xi_i + \xi_i^*)$$

subject to

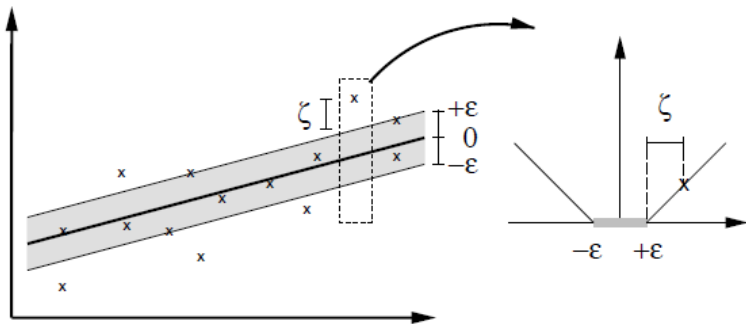
$$(y_i - \langle w, x_i \rangle - b) - \epsilon \leq \xi_i, \quad i = 1, \dots, N$$

$$(\langle w, x_i \rangle + b - y_i) - \epsilon \leq \xi_i^*, \quad i = 1, \dots, N$$

$$\xi_i \geq 0, \quad i = 1, \dots, N$$

$$\xi_i^* \geq 0, \quad i = 1, \dots, N$$

Case 1: Hyperplane



$$\min_{\mathbf{w} \in \mathbb{R}^n, b \in \mathbb{R}} \|\mathbf{w}\|^2 + C \sum_{i=1}^N (\xi_i + \xi_i^*)$$

subject to

$$\xi_i - y_i + \langle \mathbf{w}, \mathbf{x}_i \rangle + b + \epsilon \geq 0, \quad i = 1, \dots, N$$

$$\xi_i^* - \langle \mathbf{w}, \mathbf{x}_i \rangle - b + y_i + \epsilon \geq 0, \quad i = 1, \dots, N$$

$$\xi_i \geq 0, \quad i = 1, \dots, N$$

$$\xi_i^* \geq 0, \quad i = 1, \dots, N$$

Lagrangian Formulation

The Lagrangian can be written as

$$L = \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^N (\xi_i + \xi_i^*) - \sum_{i=1}^N \alpha_i (\epsilon + \xi_i - y_i + \langle \mathbf{w}, \mathbf{x}_i \rangle + b) \\ - \sum_{i=1}^N \alpha_i^* (\epsilon + \xi_i^* + y_i - \langle \mathbf{w}, \mathbf{x}_i \rangle - b) - \sum_{i=1}^N (\eta_i \xi_i + \eta_i^* \xi_i^*)$$

For $i = 1, 2, \dots, N$,

$$\alpha_i, \alpha_i^*, \eta_i, \eta_i^* \geq 0$$

KKT Conditions

$$\partial_w L = w - \sum_{i=1}^N (\alpha_i - \alpha_i^*) x_i = 0$$

$$w = \sum_{i=1}^N (\alpha_i - \alpha_i^*) x_i \quad (1)$$

$$\partial_b L = \sum_{i=1}^N (\alpha_i^* - \alpha_i) = 0 \quad (2)$$

$$\partial_{\xi_i} = C - \alpha_i - \eta_i = 0, i = 1, 2, \dots, N \quad (3)$$

$$\partial_{\xi_i^*} = C - \alpha_i^* - \eta_i^* = 0, i = 1, 2, \dots, N \quad (4)$$

KKT Complimentary Conditions

For $i = 1, 2, \dots, N$

$$\alpha_i(\epsilon + \xi_i - y_i + \langle \mathbf{w}, \mathbf{x}_i \rangle + b) = 0 \quad (5)$$

$$\alpha_i^*(\epsilon + \xi_i^* + y_i - \langle \mathbf{w}, \mathbf{x}_i \rangle - b) = 0 \quad (6)$$

$$\eta_i \xi_i = 0 \quad (7)$$

$$\eta_i^* \xi_i^* = 0 \quad (8)$$

From (3),

$$0 \leq \alpha_j \leq C \quad (9)$$

From (13),

$$0 \leq \alpha_j^* \leq C \quad (10)$$

α_j and α_j^* cannot be greater than zero at the same time.

When $\alpha_j = 0$, from (3), $\eta_j > 0$. Therefore from (7), $\xi_j = 0$
Therefore from (5),

$$\epsilon - y_i + \langle \mathbf{w}, \mathbf{x}_i \rangle + b \geq 0$$

That is

$$y_i - \langle \mathbf{w}, \mathbf{x}_i \rangle - b \leq \epsilon$$

$$H : y_i - (\langle \mathbf{w}, \mathbf{x} \rangle + b) = 0, H_1 : y_i - (\langle \mathbf{w}, \mathbf{x} \rangle + b) = \epsilon,$$

$$H_2 : (\langle \mathbf{w}, \mathbf{x} \rangle + b) - y_i = \epsilon$$

That is (x_i, y_i) lies on H or on H_1 or between H and H_1

That is, in this case, (x_i, y_i) lies on or inside ϵ - insensitive tube.

Similarly $\alpha_i^* = 0$, from (13), $\eta_i^* > 0$. Therefore from (17), $\xi_i^* = 0$
Therefore from (6),

$$\epsilon + y_i - \langle \mathbf{w}, \mathbf{x}_i \rangle - b \geq 0$$

That is

$$\langle \mathbf{w}, \mathbf{x}_i \rangle + b - y_i \leq \epsilon$$

That is (x_i, y_i) lies on H or on H_2 or between H and H_2

That is, in this case, (x_i, y_i) lies on or inside ϵ tube.

When $0 < \alpha_j < C$, from (3), $\eta_j > 0$. Therefore from (7), $\xi_j = 0$
Therefore from (5),

$$\epsilon - y_j + \langle \mathbf{w}, \mathbf{x}_j \rangle + b = 0$$

That is (\mathbf{x}_j, y_j) lies on H_1 .

When $0 < \alpha_j^* < C$, from (13), $\eta_j^* > 0$. Therefore from (17),
 $\xi_j^* = 0$

Therefore from (6),

$$\langle \mathbf{w}, \mathbf{x}_i \rangle + \mathbf{b} - y_i = \epsilon$$

That is (x_i, y_i) lies on H_2

When $\alpha_j = C$, from (3), $\eta_j = 0$. Therefore from (7), $\xi_j \geq 0$
Therefore from (5),

$$\epsilon - y_j + \langle \mathbf{w}, \mathbf{x}_j \rangle + \mathbf{b} + \xi_j = 0$$

That is

$$y_j - \langle \mathbf{w}, \mathbf{x}_j \rangle - \mathbf{b} = \epsilon + \xi_j$$

That is,

$$y_j - \langle \mathbf{w}, \mathbf{x}_j \rangle - \mathbf{b} \geq \epsilon$$

That is (\mathbf{x}_j, y_j) lies on H_1 or outside the ϵ tube

When $\alpha_j^* = C$, from (13), $\eta_j^* = 0$. Therefore from (17), $\xi_j^* \geq 0$
Therefore from (6),

$$\epsilon - \langle \mathbf{w}, \mathbf{x}_i \rangle - b + y_i + \xi_i = 0$$

That is

$$\langle \mathbf{w}, \mathbf{x}_i \rangle + b - y_i = \epsilon + \xi_i$$

That is,

$$\langle \mathbf{w}, \mathbf{x}_i \rangle + b - y_i \geq \epsilon$$

That is (x_i, y_i) lies on H_2 or outside the ϵ tube

Support Vectors

- Data with non zero coefficients in the expansion of w are called support vectors
- Support vectors lie on H_1 or on H_2 or outside the ϵ tube
- Coefficients vanish if the data points lie inside the ϵ tube

Coefficients: Primal Variable

- The terms that involve w : $\frac{1}{2}\|w\|^2 - \sum_i(\alpha_i - \alpha_i^*)\langle w, x_i \rangle$
- The terms that involve b : $b(\sum_i(\alpha_i^* - \alpha_i))$
- The terms that involve ξ_i : $\sum_{i=1}^N \xi_i(\mathbf{C} - \alpha_i - \mu_i)$
- The terms that involve ξ_i^* : $\sum_{i=1}^N \xi_i(\mathbf{C} - \alpha_i^* - \mu_i^*)$
- The terms that involve ϵ : $-\epsilon(\alpha_i + \alpha_i^*)$
- The remaining terms are: $\sum_i y_i(\alpha_i - \alpha_i^*)$

Coefficients: Primal Variable

$$\begin{aligned}\|\mathbf{w}\|^2 &= \left\langle \sum_{i=1}^N (\alpha_i - \alpha_i^*) \mathbf{x}_i, \sum_{i=1}^N (\alpha_i - \alpha_i^*) \mathbf{x}_i \right\rangle \\ &= \sum_{i=1}^N \sum_{j=1}^N (\alpha_i - \alpha_i^*) (\alpha_j - \alpha_j^*) \langle \mathbf{x}_i, \mathbf{x}_j \rangle\end{aligned}$$

$$\begin{aligned}\sum_i (\alpha_i - \alpha_i^*) \langle \mathbf{w}, \mathbf{x}_i \rangle &= \sum_i (\alpha_i - \alpha_i^*) \left\langle \sum_j (\alpha_j - \alpha_j^*) \mathbf{x}_j, \mathbf{x}_i \right\rangle \\ &= \sum_{i=1}^N \sum_{j=1}^N (\alpha_i - \alpha_i^*) (\alpha_j - \alpha_j^*) \langle \mathbf{x}_i, \mathbf{x}_j \rangle\end{aligned}$$

Dual Formulation

maximize

$$\frac{-1}{2} \sum_{i,j} (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) \langle \mathbf{x}_i, \mathbf{x}_j \rangle - \epsilon \sum_i (\alpha_i + \alpha_i^*) + \sum_i y_i (\alpha_i - \alpha_i^*)$$

subject to $\sum_i (\alpha_i - \alpha_i^*) = 0$ and $\alpha_i, \alpha_i^* \in [0, C]$.

Determination of b

Determine b using the points for which

- $0 < \alpha_j < C$
- $0 < \alpha_j^* < C$

Case II: General Form

- $\tilde{f}(x) = \langle f, k_x \rangle + b$

$$\min_{f \in \mathcal{F}, b \in \mathbb{R}} \|f\|^2 + C \sum_{i=1}^N (\xi_i + \xi_i^*)$$

subject to

$$(y_i - \langle f, k_{x_i} \rangle - b) - \epsilon \leq \xi_i, \quad i = 1, \dots, N$$

$$(\langle f, k_{x_i} \rangle + b - y_i) - \epsilon \leq \xi_i^*, \quad i = 1, \dots, N$$

$$\xi_i \geq 0, \quad i = 1, \dots, N$$

$$\xi_i^* \geq 0, \quad i = 1, \dots, N$$

$$\min_{f \in \mathcal{H}, b \in \mathbb{R}} \|f\|^2 + C \sum_{i=1}^N (\xi_i + \xi_i^*)$$

subject to

$$\xi_i - y_i + \langle f, k_{x_i} \rangle + b + \epsilon \geq 0, \quad i = 1, \dots, N$$

$$\xi_i^* - \langle f, k_{x_i} \rangle - b + y_i + \epsilon \geq 0, \quad i = 1, \dots, N$$

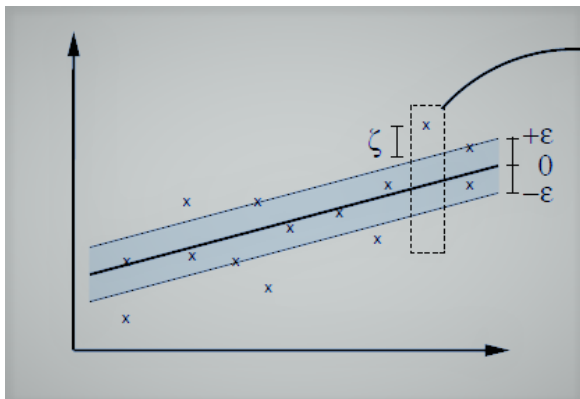
$$\xi_i \geq 0, \quad i = 1, \dots, N$$

$$\xi_i^* \geq 0, \quad i = 1, \dots, N$$

Hyperplane: RKHS

$$H : y_i - (\langle f, k_{x_i} \rangle + b) = 0, H_1 : y_i - (\langle f, k_{x_i} \rangle + b) = \epsilon,$$

$$H_2 : (\langle f, k_{x_i} \rangle + b) - y_i = \epsilon$$



Lagrangian Formulation

The Lagrangian can be written as

$$L = \frac{1}{2} \|f\|^2 + C \sum_{i=1}^N (\xi_i + \xi_i^*) - \sum_{i=1}^N \alpha_i (\epsilon + \xi_i - y_i + \langle f, k_{x_i} \rangle + b) \\ - \sum_{i=1}^N \alpha_i^* (\epsilon + \xi_i^* + y_i - \langle f, k_{x_i} \rangle - b) - \sum_{i=1}^N (\eta_i \xi_i + \eta_i^* \xi_i^*)$$

For $i = 1, 2, \dots, N$,

$$\alpha_i, \alpha_i^*, \eta_i, \eta_i^* \geq 0$$

KKT Conditions

$$\partial_f L = f - \sum_{i=1}^N (\alpha_i - \alpha_i^*) k_{x_i} = 0$$

$$f = \sum_{i=1}^N (\alpha_i - \alpha_i^*) k_{x_i} \quad (11)$$

$$\partial_b L = \sum_{i=1}^N (\alpha_i^* - \alpha_i) = 0 \quad (12)$$

$$\partial_{\xi_i} = C - \alpha_i - \eta_i = 0, i = 1, 2, \dots, N \quad (13)$$

$$\partial_{\xi_i^*} = C - \alpha_i^* - \eta_i^* = 0, i = 1, 2, \dots, N \quad (14)$$

KKT Complimentary Conditions

For $i = 1, 2, \dots, N$

$$\alpha_i(\epsilon + \xi_i - y_i + \langle f, k_{x_i} \rangle + b) = 0 \quad (15)$$

$$\alpha_i^*(\epsilon + \xi_i^* + y_i - \langle f, k_{x_i} \rangle - b) = 0 \quad (16)$$

$$\eta_i \xi_i = 0 \quad (17)$$

$$\eta_i^* \xi_i^* = 0 \quad (18)$$

$\alpha_i \alpha_i^* = 0$, there can never be a set of dual variables α_i, α_i^* which are both simultaneously nonzero.

From (13),

$$0 \leq \alpha_j \leq C \quad (19)$$

From (14),

$$0 \leq \alpha_j^* \leq C \quad (20)$$

α_j and α_j^* cannot be greater than zero at the same time.

When $\alpha_j = 0$, from (13), $\eta_j > 0$. Therefore from (17), $\xi_j = 0$
Therefore from (15),

$$\epsilon - y_i + \langle \mathbf{f}, \mathbf{k}_{x_i} \rangle + b \geq 0$$

That is

$$y_i - \langle \mathbf{f}, \mathbf{k}_{x_i} \rangle - b \leq \epsilon$$

That is (\mathbf{k}_{x_i}, y_i) lies on H or on H_1 or between H and H_1

That is, in this case, (\mathbf{k}_{x_i}, y_i) lies on or inside ϵ -insensitive tube.

Similarly when $\alpha_j^* = 0$, from (14), $\eta_j^* > 0$. Therefore from (18),
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Therefore from (15),

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That is (k_{x_i}, y_i) lies on H_1 .

When $0 < \alpha_j^* < C$, from (14), $\eta_j^* > 0$. Therefore from (18), $\xi_j^* = 0$.

Therefore from (16),

$$\langle \mathbf{f}, \mathbf{k}_{x_i} \rangle + \mathbf{b} - y_i = \epsilon$$

That is (\mathbf{k}_{x_i}, y_i) lies on H_2 .

When $\alpha_j = C$, from (13), $\eta_j = 0$. Therefore from (17), $\xi_j \geq 0$
Therefore from (15),

$$\epsilon - y_i + \langle f, k_{x_i} \rangle + b + \xi_i = 0$$

That is

$$y_i - \langle f, k_{x_i} \rangle - b = \epsilon + \xi_i$$

That is,

$$y_i - \langle f, k_{x_i} \rangle - b \geq \epsilon$$

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When $\alpha_j^* = C$, from (14), $\eta_j^* = 0$. Therefore from (18), $\xi_j^* \geq 0$
Therefore from (16),

$$\epsilon - \langle \mathbf{f}, \mathbf{k}_{x_i} \rangle - \mathbf{b} + y_i + \xi_i^* = 0$$

That is

$$\langle \mathbf{f}, \mathbf{k}_{x_i} \rangle + \mathbf{b} - y_i = \epsilon + \xi_i^*$$

That is,

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Support Vectors

- Data with non zero coefficients in the expansion of f are called support vectors
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Coefficients: Primal Variable

$$\begin{aligned}\|f\|^2 &= \left\langle \sum_{i=1}^N (\alpha_i - \alpha_i^*) \mathbf{k}_{x_i}, \sum_{i=1}^N (\alpha_i - \alpha_i^*) \mathbf{k}_{x_i} \right\rangle \\ &= \sum_{i=1}^N \sum_{j=1}^N (\alpha_i - \alpha_i^*) (\alpha_j - \alpha_j^*) \langle \mathbf{k}_{x_i}, \mathbf{k}_{x_j} \rangle\end{aligned}$$

$$\begin{aligned}\sum_i (\alpha_i - \alpha_i^*) \langle f, \mathbf{k}_{x_i} \rangle &= \sum_i (\alpha_i - \alpha_i^*) \left\langle \sum_j (\alpha_j - \alpha_j^*) \mathbf{k}_{x_j}, \mathbf{k}_{x_i} \right\rangle \\ &= \sum_{i=1}^N \sum_{j=1}^N (\alpha_i - \alpha_i^*) (\alpha_j - \alpha_j^*) \langle \mathbf{k}_{x_i}, \mathbf{k}_{x_j} \rangle\end{aligned}$$

Dual Formulation

maximize

$$\frac{-1}{2} \sum_{i,j} (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) \langle \mathbf{k}_{x_i}, \mathbf{k}_{x_j} \rangle - \epsilon \sum_i (\alpha_i + \alpha_i^*) + \sum_i y_i (\alpha_i - \alpha_i^*)$$

subject to $\sum_i (\alpha_i - \alpha_i^*) = 0$ and $\alpha_i, \alpha_i^* \in [0, C]$.

Determination of b

Determine b using the points for which

- $0 < \alpha_j < C$
- $0 < \alpha_j^* < C$