Support vector machines

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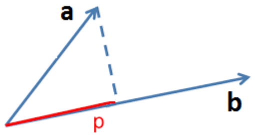
Reminder

1. $a = [a^1, ...a^D]^T$, $b = [b^1, ...b^D]^T$
2. Scalar product $\langle a, b\rangle = a^T b = \sum_{d=1}^{D} a_d b_b$
3. $a \perp b$ means that $\langle a, b\rangle = 0$
4. Norm $\|a\| = \sqrt{\langle a, a\rangle}$
5. Distance $\rho(a, b) = \|a - b\| = \sqrt{\langle a - b, a - b\rangle}$



- $p = \langle a, \frac{b}{\|b\|}\rangle$
- $|p| = \left|a, \frac{b}{\|b\|}\right|$- unsigned projection length

Orthogonal vector to hyperplane

Theorem 1

Vector w is orthogonal to hyperplane $w^T x + w_0 = 0$

Proof. Consider arbitrary $x_A, x_B \in \{x : \ w^T x + w_0 = 0\}$:

$$w^T x_A + w_0 = 0 \tag{1}$$

$$w^T x_B + w_0 = 0 \tag{2}$$

By substracting (2) from (1), obtain $w^T(x_A - x_B) = 0$, so w is orthogonal to hyperplane. □

Distance from point to hyperplane

Theorem 2

Distance from point x to hyperplane $w^T x + w_0 = 0$ is equal to $\frac{w^T x + w_0}{\|w_0\|}$.

Proof. Project x on the hyperplane, let the projection be p and complement $h = x - p$, orthogonal to hyperplane. Then

$$x = p + h$$

Since p lies on the hyperplane,

$$w^T p + w_0 = 0$$

Since h is orthogonal to hyperplane and according to theorem 1

$$h = r\frac{w}{\|w\|},\ r \in \mathbb{R} \text{ - distance to hyperplane.}$$

Distance from point to hyperplane

$$x = p + r\frac{w}{\|w\|}$$

After multiplication by w and addition of w_0:

$$w^T x + w_0 = w^T p + w_0 + r\frac{w^T w}{\|w\|} = r\|w\|$$

because $w^T p + w_0 = 0$ and $\|w\| = \sqrt{w^T w}$. So we get, that

$$r = \frac{w^T x + w_0}{\|w\|}$$

Comments:

- From one side of hyperplane $r > 0 \Leftrightarrow w^T x + w_0 > 0$
- From the other side $r < 0 \Leftrightarrow w^T x + w_0 < 0$.
- Distance from hyperplane to origin 0 is $\frac{w_0}{\|w\|}$. So w_0 accounts for hyperplane offset.

Binary linear classifier geometric interpretation

Binary linear classifier:

$$\widehat{y}(x) = \text{sign}\left(w^T x + w_0\right)$$

divides feature space by hyperplane $w^T x + w_0 = 0$.

- Confidence of decision is proportional to distance to hyperplane $\frac{|w^T x + w_0|}{\|w\|}$.
- $w^T x + w_0$ is the confidence that class is positive.

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Support vector machines

(a) (b)

Support vector machines

(a) (b)

Main idea

Select hyperplane maximizing the spread between classes.

Support vector machines

Objects x_i for $i = 1, 2, ...n$ lie at distance $b/|w|$ from discriminant hyperplane if

$$\begin{cases} x_i^T w + w_0 \geq b, & y_i = +1 \\ x_i^T w + w_0 \leq -b & y_i = -1 \end{cases} \quad i = 1, 2, ...N.$$

This can be rewritten as

$$y_i(x_i^T w + w_0) \geq b, \quad i = 1, 2, ...N.$$

The margin is equal to $2b/\|w\|$. Since w, w_0 and b are defined up to multiplication constant, we can set $b = 1$.

Problem statement

Problem statement:

$$\begin{cases} \frac{1}{2}w^T w \to \min\limits_{w,w_0} \\ y_i(x_i^T w + w_0) \ge 1, \quad i = 1, 2, ...N. \end{cases}$$

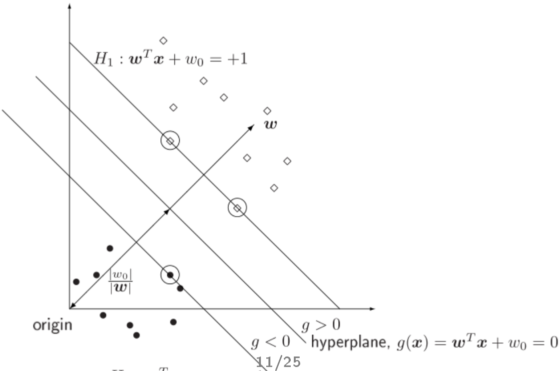
Support vectors

non-informative observations: $y_i(x_i^T w + w_0) > 1$

- do not affect the solution

support vectors: $y_i(x_i^T w + w_0) = 1$

- lie at distance $1/\|w\|$ to separating hyperplane
- affect the the solution.



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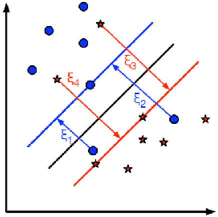
Linearly non-separable case



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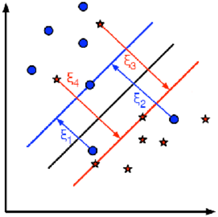
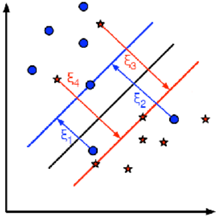


$$\begin{cases} \frac{1}{2}w^T w \to \min\limits_{w,w_0} \\ y_i(x_i^T w + w_0) \geq 1, \quad i = 1, 2, ...N. \end{cases}$$

Linearly non-separable case



$$\begin{cases} \frac{1}{2}w^T w \to \min\limits_{w, w_0} \\ y_i(x_i^T w + w_0) \geq 1, \quad i = 1, 2, \ldots N. \end{cases}$$

Problem

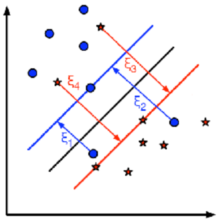
Constraints become incompatible and give empty set!

Linearly non-separable case

No separating hyperplane exists. Errors are permitted by including slack variables ξ_i:

$$\begin{cases} \frac{1}{2}w^T w + C\sum_{i=1}^N \xi_i \to \min_{w,\xi} \\ y_i(w^T x_i + w_0) \geq 1 - \xi_i,\ i = 1, 2, \ldots N \\ \xi_i \geq 0,\ i = 1, 2, \ldots N \end{cases}$$

- Parameter C is the cost for misclassification and controls the bias-variance trade-off.
- It is chosen on validation set.
- Other penalties are possible, e.g. $C\sum_i \xi_i^2$.



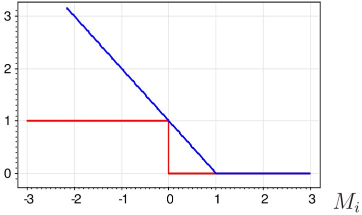
Classification of training objects

- **Non-informative objects**:
  - $y_i(w^T x_i + w_0) > 1$
- **Support vectors** SV**:**
  - $y_i(w^T x_i + w_0) \le 1$
  - **boundary support vectors** $\widetilde{SV}$:
    - $y_i(w^T x_i + w_0) = 1$
  - **violating support vectors**:
    - $y_i(w^T x_i + w_0) > 0$: violating support vector is correctly classified.
    - $y_i(w^T x_i + w_0) < 0$: violating support vector is misclassified.

SVM with unconstrained optimization

Optimization problem:

$$\begin{cases} \frac{1}{2}w^T w + C\sum_{i=1}^N \xi_i \to \min_{w,w_0,\xi} \\ y_i(w^T x_i + w_0) = M_i(w,w_0) \ge 1 - \xi_i, \\ \xi_i \ge 0,\ i = 1,2,...N \end{cases}$$



can be rewritten as

$$\frac{1}{2C}\left\lVert w\right\rVert_2^2 + \sum_{i=1}^N [1 - M_i(w,w_0)]_+ \to \min_{w,w_0,\xi}$$

Thus SVM is linear discriminant function with cost approximated with $\mathcal{L}(M) = [1-M]_+$ and L_2 regularization.

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Dual problem

Solving Karush-Kuhn-Takker conditions, get **dual optimization problem**:

$$\begin{cases} L_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^T x_j \to \max_\alpha \\ \sum_{n=1}^{N} \alpha_n y_n = 0 \\ 0 \le \alpha_n \le C, \quad n = \overline{1, N} \end{cases} \tag{3}$$

It is standard quadratic programming task.

Comments on support vectors

- **non-informative vectors**: $y_i(w^T x_i + w_0) > 1$ have $\alpha_i = 0$
- **non-boundary support vectors** $SV \setminus \tilde{SV}$:
  $y_i(w^T x_i + w_0) < 1$ have $\alpha_i = C$.
- **boundary support vectors** $\widetilde{\mathcal{SV}}$: $y_i(w^T x_i + w_0) = 1$
  Typically $\alpha_i \in (0, C)$, though $\alpha_i = 0, C$ are possible as special cases.

Solution

1. Solve (3) to find optimal dual variables α_i^*
2. Find optimal w ($\alpha_i^* \neq 0$ only for support vectors):
$$w = \sum_{i \in \mathcal{SV}} \alpha_i^* y_i x_i$$
3. w_0 can be found from any edge equality for boundary support vector:
$$y_i(x_i^T w + w_0) = 1,\ \forall i \in \widetilde{\mathcal{SV}} \tag{4}$$

Solution for w_0

By multiplyting (4) by y_i obtain

$$x_i^T w + w_0 = y_i \quad \forall i \in \widetilde{\mathcal{SV}} \tag{5}$$

Get more numerically stable from summing 5 over all $i \in \widetilde{\mathcal{SV}}$:

$$n_{\tilde{SV}} w_0 = \sum_{j \in \tilde{SV}} \left(y_j - x_j^T w \right) = \sum_{j \in \tilde{SV}} y_j - \sum_{j \in \tilde{SV}} x_j^T w, \quad n_{\tilde{SV}} = \left| \tilde{SV} \right|$$

$$w_0 = \frac{1}{n_{\tilde{SV}}} \left(\sum_{j \in \tilde{SV}} y_j - \sum_{j \in \tilde{SV}} \overbrace{\sum_{i \in \mathcal{SV}} \alpha_i^* y_i x_i^T}^{w^T} x_j \right)$$

If there exist no boundary support vectors (only violating SV), then find w_0 by grid search.

Making predictions

1. Solve dual task to find α_i^*, $i = 1, 2, ...N$

$$\begin{cases} \sum_{i=1}^N \alpha_i - \frac{1}{2}\sum_{i=1}^N \sum_{j=1}^N \alpha_i\alpha_j y_i y_j \langle x_i, x_j\rangle \to \max_\alpha \\ \sum_{i=1}^N \alpha_i y_i = 0 \\ 0 \le \alpha_i \le C \quad \text{(using (??) and that } \alpha_i \ge 0,\ r_i \ge 0) \end{cases}$$

2. Find optimal w_0:

$$w_0 = \frac{1}{n_{\tilde{SV}}}\left(\sum_{j\in\tilde{SV}} y_j - \sum_{j\in\tilde{SV}}\sum_{i\in\mathcal{SV}} \alpha_i^* y_i \langle x_i, x_j\rangle\right)$$

3. Make prediction for new x:

$$\hat{y} = \text{sign}[w^T x + w_0] = \text{sign}[\sum_{i\in\mathcal{SV}} \alpha_i^* y_i \langle x_i, x\rangle + w_0]$$

Making predictions

1. Solve dual task to find α_i^*, $i = 1, 2, ...N$

$$\begin{cases} L_D = \sum_{i=1}^N \alpha_i - \frac{1}{2}\sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle \to \max_\alpha \\ \sum_{i=1}^N \alpha_i y_i = 0 \\ 0 \le \alpha_i \le C \quad \text{(using (??) and that } \alpha_i \ge 0,\ r_i \ge 0) \end{cases}$$

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- On all steps we don't need exact feature representations, only scalar products $\langle x, x' \rangle$!

Kernel trick generalization

1. Solve dual task to find α_i^*, $i = 1, 2, ...N$

$$\begin{cases} L_D = \sum_{i=1}^N \alpha_i - \frac{1}{2}\sum_{i=1}^N \sum_{j=1}^N \alpha_i\alpha_j y_i y_j K(x_i, x_j) \to \max_\alpha \\ \sum_{i=1}^N \alpha_i y_i = 0 \\ 0 \le \alpha_i \le C \end{cases}$$

2. Find optimal w_0:

$$w_0 = \frac{1}{n_{\tilde{SV}}}\left(\sum_{j\in\tilde{SV}} y_j - \sum_{j\in\tilde{SV}}\sum_{i\in\mathcal{SV}} \alpha_i^* y_i K(x_i, x_j)\right)$$

3. Make prediction for new x:

$$\widehat{y} = \text{sign}[w^T x + w_0] = \text{sign}[\sum_{i\in\mathcal{SV}} \alpha_i^* y_i K(x_i, x) + w_0]$$

- We replaced $\langle x, x'\rangle \to K(x, x')$ for $K(x, x') = \langle\phi(x), \phi(x')\rangle$ for some feature transformation $\phi(\cdot)$.

Summary

- SVM - linear classifier with L_2 regularization and hinge loss.
- Geometrically SVM maximizes border between classes.
- Solution depends only on support vectors, having margin≤ 1.
- Solution depends on x only through $\langle x_i, x_j\rangle$
    - may generalize $\langle x_i, x_j\rangle$ to $K(x_i, x_j)$.