Support vector machines

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Support vector machines

(a) (b)

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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:

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

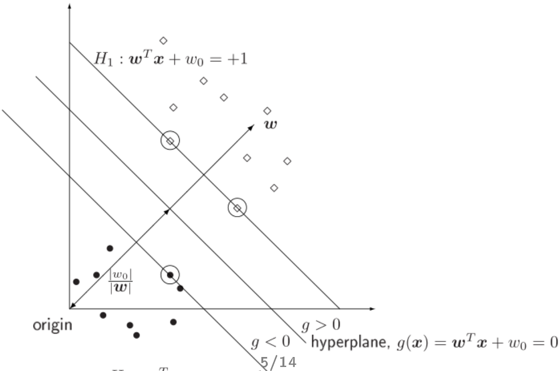
Support vectors

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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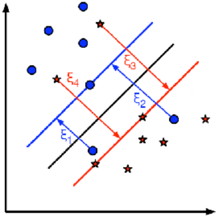
Linearly non-separable case



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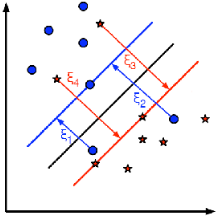
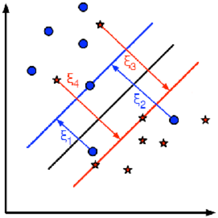


$$\begin{cases} \frac{1}{2} w^T w \to \min\limits_{w, w_0} \\ y_i(x_i^T w + w_0) \geq 1, \quad i = 1, 2, \dots N. \end{cases}$$

Linearly non-separable case



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

Problem

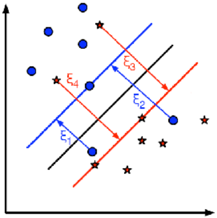
Constraints become incompatible and give empty set!

Linearly non-separable case

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

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

- 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:
  - $y_i(w^T x_i + w_0) \leq 1$
  - **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.

Solution of linearly non-separable case

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

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

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^*, $i = 1, 2, ... N$

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

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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^*, $i = 1, 2, \dots N$

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

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:

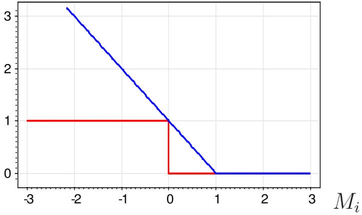
$$\widehat{y} = \text{sign}[w^T x + w_0] = \text{sign}[\sum_{i \in \mathcal{SV}} \alpha_i^* y_i K(x_i, x_j) + w_0]$$

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

Another view on SVM

Optimization problem:

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



can be rewritten as

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

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

Sparsity of solution

- SVM solution depends only on support vectors
- This is also clear from loss function, satisfying $\mathcal{L}(M) = 0$ for $M \geq 1$.
    - objects with margin≥ 1 don't affect solution!
- Sparsity causes SVM to be less robust to outliers
    - because outliers are always support vectors