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

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

This can be rewritten as

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

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:

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

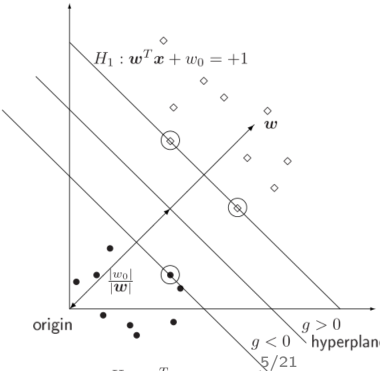
Support vectors

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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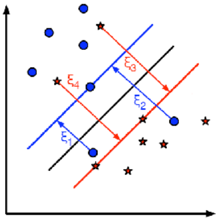
Linearly non-separable case



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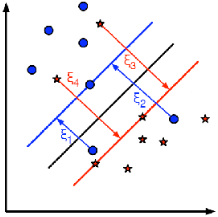
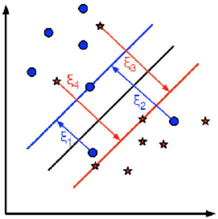


$$\begin{cases} \frac{1}{2}w^T w \to \min_{w,w_0} \\ y_i(x_i^T w + w_0) \geq 1, \quad i = 1, 2, \ldots N. \end{cases}$$

Linearly non-separable case



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

Problem

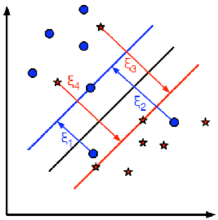
Constraints become incompatible and give empty set!

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. $C\sum_i \xi_i^2$.



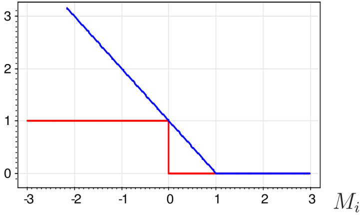
Classification of training objects

- **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.

SVM with unconstrained optimization

Optimization problem:

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



can be rewritten as

$$\frac{1}{2C}\|w\|_2^2 + \sum_{i=1}^{N}[1-M_i(w,w_0)]_+ \to \min_{w,w_0,\xi}$$

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

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

Multiclass SVM

C discriminant functions are built simultaneously:

$$g_c(x) = (\mathbf{w}^c)^T x + w_0^c, \qquad c = \overline{1, C}.$$

Linearly separable case:

$$\begin{cases} \sum_{c=1}^{C} (\mathbf{w}^c)^T \mathbf{w}^c \to \min_{\mathbf{w}} \\ (\mathbf{w}^{y_n})^T x_n + w_0^{y_n} - (\mathbf{w}^c)^T x - w_0^c \geq 1 \quad \forall c \neq y_n, \\ n = \overline{1, N}. \end{cases}$$

Linearly non-separable case:

$$\begin{cases} \sum_{c=1}^{C} (\mathbf{w}^c)^T \mathbf{w}^c + C \sum_{n=1}^{N} \xi_n \to \min_w \\ (\mathbf{w}^{y_n})^T x + w_0^{y_n} - (\mathbf{w}^c)^T x - w_0^c \geq 1 - \xi_n \quad \forall c \neq y_n, \\ \xi_n \geq 0, \quad n = \overline{1, N}. \end{cases}$$

Is slower, but shows similar accuracy to one-vs-all,one-vs-one SVM.

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Dual problem

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

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

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 (1) 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:

$$y_i(x_i^T w + w_0) = 1, \forall i \in \widetilde{\mathcal{SV}} \qquad (2)$$

Solution for w_0

By multiplyting (2) by y_i obtain

$$x_i^T w + w_0 = y_i \quad \forall i \in \widetilde{\mathcal{SV}} \tag{3}$$

Get more numerically stable from summing 3 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^*, $i = 1, 2, \dots N$

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

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:

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

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

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

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:

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

- 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 $K(x_i, x_j)$.