Support vector machines

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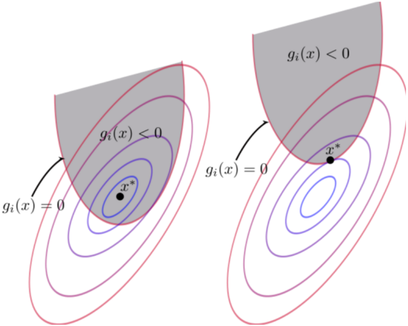
Kuhn-Takker conditions

Consider the optimization task:

$$\begin{cases} f(x) \to \min_x \\ g_m(x) \le 0 \qquad m = \overline{1, M} \end{cases} \tag{1}$$



Necessary conditions for optimality

Define Largangian

$$L(x, \lambda) = f(x) + \sum_{m=1}^{M} \lambda_m g_m(x)$$

Theorem (necessary conditions for optimality):

- Let x^* be the solution to (1),
- $f(x^*)$ and $g_m(x^*)$, $m = 1, 2, ...M$ - continuously differentiable at x^*.
- Slater regularity satisfied: $\exists x : \; g_m(x) < 0 \, \forall m$.

Then coefficients $\lambda_1^*, \lambda_2^*, ...\lambda_M^*$ exist, such that x^* satisfies the conditions for $m = \overline{1, M}$:

$$\begin{cases} \nabla_x f(x^*) + \sum_{i=1}^{M} \lambda_i^* \nabla_x g_i(x^*) = 0 & \text{stationarity} \\ g_m(x^*) \le 0 & \text{feasibility} \\ \lambda_m^* \ge 0 & \text{non-negativity} \\ \lambda_m^* g_m(x^*) = 0 & \text{comp.slackness} \end{cases} \tag{2}$$

Kuhn-Takker conditions

- Suppose $f(x)$ and $g_m(x)$, $m=\overline{1,M}$ are convex. Then
  1. Kuhn-Takker conditions (2) become **sufficient** for x^* to be the solution of (1).
  2. (x^*,λ^*) form the **saddle point for Lagrangian**:

$$L(x^*,\lambda)\le L(x^*,\lambda^*)\le L(x,\lambda^*)\quad\forall x\,\forall\lambda\in\mathbb{R}_+^M$$

  3. May find $x^*=x(\lambda^*)$ from $\nabla_x L(x^*,\lambda^*)=0$. Since $L(x^*,\lambda^*)$ is saddle point, find λ^* from dual task:

$$\begin{cases}L(x(\lambda),\lambda)\to\max_\lambda & \\ g_m(x(\lambda))\le 0 & m=\overline{1,M}\\ \lambda_m\ge 0 & m=\overline{1,M}\\ \lambda_m g_m(x(\lambda))=0 & m=\overline{1,M}\end{cases}$$

Convex optimization

Why convexity of $f(x)$ and $g_m(x)$, $m = \overline{1, M}$ is convenient:

- All local minimums become global minimums
- The set of minimums is convex
- If $f(x)$ is strictly convex and minimum exists, then it is unique.

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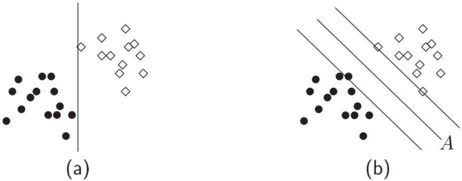
Support vector machines



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 $b/\left\|w\right\|$ 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

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

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

Problem statement

Problem statement:

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

Problem statement

Problem statement:

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

Lagrangian:

$$L = \frac{1}{2}w^T w - \sum_{i=1}^{N} \alpha_i (y_i(w^T x + w_0) - 1)$$

By Karush-Kuhn-Takker the solution satisfies:

$$\begin{cases} \frac{\partial L}{\partial w} = \mathbf{0}, \ \frac{\partial L}{\partial w_0} = 0 \\ y_i(x_i^T w + w_0) - 1 \geq 0, \\ \alpha_i(y_i(x_i^T w + w_0) - 1) = 0, \\ \alpha_i \geq 0, \quad i = 1, 2, ...N \end{cases}$$

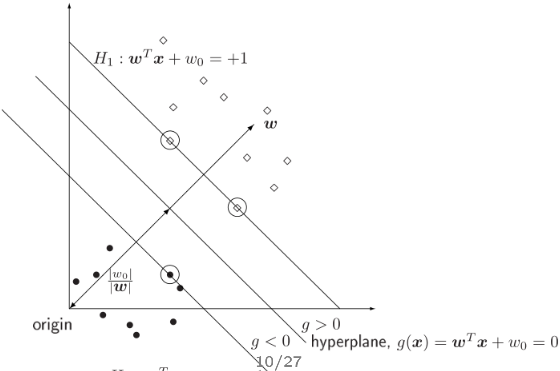
Support vectors

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

- do not affect the solution

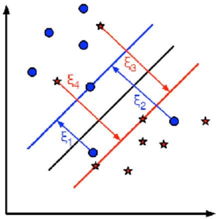
support vectors: $y_i(x_i^T w + w_0) = 1$

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

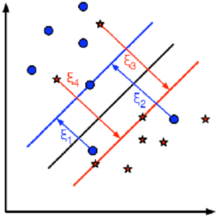


2. Linearly separable SVM
   - Linearly non-separable case

Linearly non-separable case

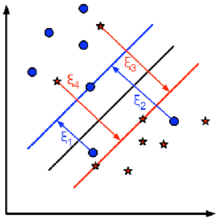


Linearly non-separable case



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

Linearly non-separable case



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

Problem

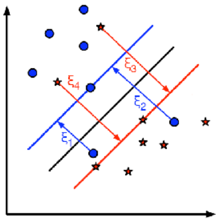
Constraints become incompatible and give empty set!

Linearly non-separable case

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

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

- 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. $C\sum_i \xi_i^2$.



Linearly non-separable case

Lagrangian:

$$L = \frac{1}{2} w^T w + C \sum_i \xi_i - \sum_{i=1}^{N} \alpha_i (y_i (w^T x_i + w_0) - 1 + \xi_i) - \sum_{i=1}^{N} r_i \xi_i$$

By Karush-Kuhn-Takker conditions, the solution satisfies constraints:

$$\begin{cases} \frac{\partial L_P}{\partial w} = \mathbf{0}, \ \frac{\partial L_P}{\partial w_0} = 0, \ \frac{\partial L_P}{\partial \xi_i} = 0 \\ \xi_i \geq 0, \ \alpha_i \geq 0, \ r_i \geq 0 \\ y_i (x_i^T w + w_0) \geq 1 - \xi_i, \\ \alpha_i (y_i (w^T x_i + w_0) - 1 + \xi_i) = 0 \\ r_i \xi_i = 0, \quad i = 1, 2, \ldots N \end{cases}$$

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.

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Solving Karush-Kuhn-Takker conditions

$$\frac{\partial L}{\partial w} = \mathbf{0}: \; w = \sum_{i=1}^{N} \alpha_i y_i x_i \tag{3}$$

$$\frac{\partial L}{\partial w_0} = 0: \; \sum_{i=1}^{N} \alpha_i y_i = 0$$

$$\frac{\partial L}{\partial \xi_i} = 0: \; C - \alpha_i - r_i = 0 \tag{4}$$

Substituting these constraints into L, we obtain the *dual problem*[1]:

$$\begin{cases} L_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^T x_j \to \max_\alpha \\ \sum_{i=1}^{N} \alpha_i y_i = 0 \\ 0 \le \alpha_i \le C \quad \text{(using (4) and that } \alpha_i \ge 0,\ r_i \ge 0) \end{cases} \tag{5}$$

[1] Dual Lagrangian is maximized because original Lagrangian has saddlepoint in optimum, min for w, w_0, ξ_i and max for α_i, r_i.

Comments on support vectors

- **non-informative vectors**: $y_i(w^T x_i + w_0) > 1 <=> \xi_i = 0$, $y_i(w^T x_i + w_0) - 1 + \xi_i > 0 => \alpha_i = 0$
  - support vectors SV will have $\alpha_i > 0$.
- **non-boundary support vectors** $SV \setminus \tilde{SV}$: $y_i(w^T x_i + w_0) < 1 <=> \xi_i > 0 => r_i = 0 <=> \alpha_i = C$.
- **boundary support vectors** $\widetilde{\mathcal{SV}}$: $y_i(w^T x_i + w_0) = 1 =>$
  - $\xi_i = 0 =>$ typically $r_i > 0 =>$ typically $\alpha_i < C$
  - $y_i(w^T x_i + w_0) - 1 + \xi_i = 0 =>$ typically $\alpha_i > 0$

  So typically $\alpha_i \in (0, C)$, though $\alpha_i = 0, C$ may appear as special case.

Solution

1. Solve (5) to find optimal dual variables α_i^*
2. Using (3) and that $\alpha_i^* = 0$ for non support vectors, find optimal w

$$w = \sum_{i \in \mathcal{SV}} \alpha_i^* y_i x_i$$

3. w_0 can be found from any edge equality for boundary support vector:

$$y_i(x_i^T w + w_0) = 1, \forall i \in \widetilde{\mathcal{SV}} \tag{6}$$

Solution for w_0

By multiplyting (6) by y_i obtain

$$x_i^T w + w_0 = y_i \quad \forall i \in \widetilde{\mathcal{SV}} \tag{7}$$

Get more numerically stable from summing 7 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^*, $i = 1, 2, ... N$

$$\begin{cases} \sum_{i=1}^N \alpha_i - \frac{1}{2}\sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle \to \max_\alpha \\ \sum_{i=1}^N \alpha_i y_i = 0 \\ 0 \le \alpha_i \le C \quad \text{(using (4) and that } \alpha_i \ge 0,\ r_i \ge 0) \end{cases}$$

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

$$\begin{cases} L_D = \sum_{i=1}^N \alpha_i - \frac{1}{2}\sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle \to \max_\alpha \\ \sum_{i=1}^N \alpha_i y_i = 0 \\ 0 \le \alpha_i \le C \quad \text{(using (4) and that } \alpha_i \ge 0,\ r_i \ge 0) \end{cases}$$

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

$$\begin{cases} L_D = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j K(x_i, x_j) \to \max_\alpha \\ \sum_{i=1}^N \alpha_i y_i = 0 \\ 0 \le \alpha_i \le C \quad \text{(using (4) and that } \alpha_i \ge 0,\ r_i \ge 0) \end{cases}$$

2. Find optimal w_0:

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

3. Make prediction for new x:

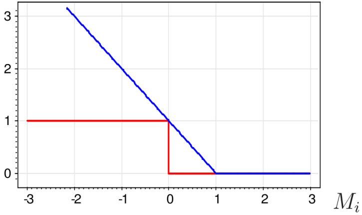
$$\hat{y} = \text{sign}[w^T x + w_0] = \text{sign}[\sum_{i \in \mathcal{SV}} \alpha_i^* y_i K(x_i, x) + w_0]$$

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

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

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

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.

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 $K(x_i, x_j)$.