Support Vector Machine (SVM)

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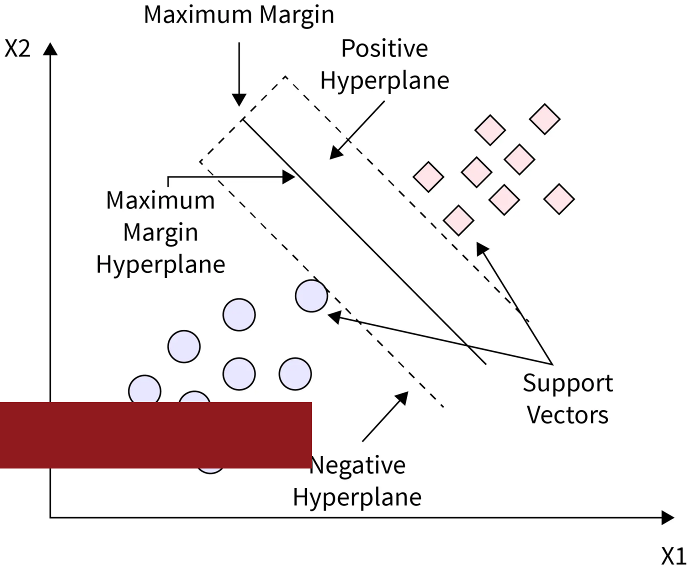
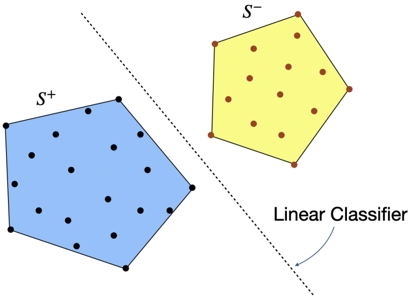


Linear Classifier

Linear separability

Consider a dataset $S = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ such that $x_i \in \mathbb{R}^m$ and $y_i \in \{-1, +1\}$ for all i. Define $S^+ = (x \mid (x, y) \in S\ ,\ \ y = +1)$ and $S^- = (x \mid (x, y) \in S\ ,\ \ y = -1)$.

Suppose that $\mathsf{Co}(S^+) \cap \mathsf{Co}(S^-) = \emptyset$. Hence, $\exists$ a hyperplane $f(x) := w^\intercal x + b$ such that $f(x) > 0\ , \forall x \in S^+$ and $f(x) < 0\ , \forall x \in S^-$.



Determining a linear classifier

Determining $(w, b) \in \mathbb{R}^m \times \mathbb{R}$ such that $\text{sign}(w^\intercal x + b) > 0$ for all $x \in S^+$ and $\text{sign}(w^\intercal x + b) < 0$ for all $x \in S^-$ reduces to the following LP:

$$\begin{array}{ll} \underset{w \in \mathbb{R}^m,\ b \in \mathbb{R}}{\text{Minimize}} & 1 \\ \text{Subject to} & y_i(w^\intercal x_i + b) > 0 \quad ,\ i = 1, \ldots, n \end{array}$$

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There can be infinitely many solutions to the above optimization problem.

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SVM. Determine $(w, b) \in \mathbb{R}^m \times \mathbb{R}$ that maximizes the **separation margin**. That is, on top of satisfying the separation constraint, we would like to

$$\text{Maximize} \min_{i=1,\ldots,n} \frac{|w^\intercal x_i + b|}{\|w\|}$$

Linear SVM

$$
\begin{aligned}
&\underset{w\in\mathbb{R}^m,\ b\in\mathbb{R}}{\text{Maximize}} && \min_{i=1,\dots,n} \frac{|w^\intercal x_i + b|}{\|w\|} \\
&\text{Subject to} && y_i(w^\intercal x_i + b) > 0 \qquad , \ i = 1, \dots, n
\end{aligned}
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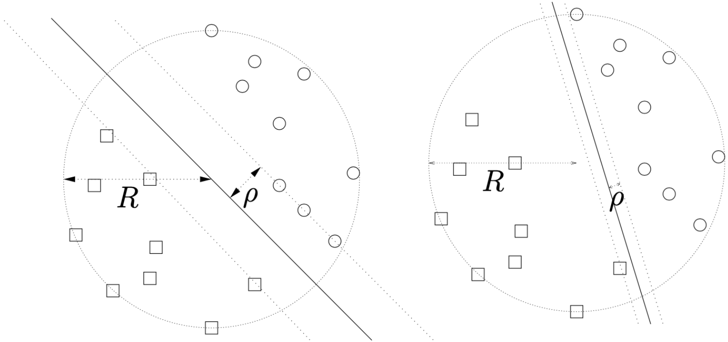

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Is the above a convex optimization problem?

Linear SVM

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Is the above a convex optimization problem?

No.

Linear SVM

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\end{aligned}$$

We can reduce the above to the following:

$$\begin{aligned}
\underset{\rho\in\mathbb{R},\ w\in\mathbb{R}^m,\ b\in\mathbb{R}}{\text{Maximize}} \quad & \frac{\rho}{\|w\|} \\
\text{Subject to} \quad & y_i(w^\intercal x_i + b) > 0 \quad , \ i = 1, \dots, n \\
& |w^\intercal x_i + b| \geq \rho \qquad , \ i = 1, \dots, n \\
& \rho > 0
\end{aligned}$$

Linear SVM

$$\begin{array}{ll} \underset{w\in\mathbb{R}^m,\ b\in\mathbb{R}}{\text{Maximize}} & \min_{i=1,\dots,n} \frac{|w^\intercal x_i + b|}{\|w\|} \\ \text{Subject to} & y_i(w^\intercal x_i + b) > 0 \qquad , \ i = 1, \dots, n \end{array}$$

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This can be further reduced to (why?):

$$\begin{array}{ll} \underset{\rho\in\mathbb{R},\ w\in\mathbb{R}^m,\ b\in\mathbb{R}}{\text{Maximize}} & \frac{\rho}{\|w\|} \\ \text{Subject to} & y_i(w^\intercal x_i + b) \geq \rho \quad , \ i = 1, \dots, n \\ & \rho > 0 \end{array}$$

Linear SVM as quadratic optimization problem

Recall that $\rho > 0$. Define $(w', b') = \frac{1}{\rho}(w, b)$. With this substitution, we obtain that

$$
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is reducible to

$$\begin{array}{ll} \underset{w\in\mathbb{R}^m,\ b\in\mathbb{R}}{\text{Maximize}} & \frac{1}{\|w\|} \\ \text{Subject to} & y_i(w^\intercal x_i + b) \geq 1 \quad , \ i = 1, \ldots, n \end{array}$$

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This can be solved using the following **quadratic programming** (QP):

$$\begin{aligned} \underset{w\in\mathbb{R}^m,\ b\in\mathbb{R}}{\text{Minimize}} \quad & \frac{1}{2}\|w\|^2 \\ \text{Subject to} \quad & 1 - y_i(w^\intercal x_i + b) \leq 0 \quad , \ i = 1, \dots, n \end{aligned} \tag{Linear SVM}$$

Lagrange dual of linear SVM

Lagrange dual function:

$$\mathcal{L}(w, b, \lambda) := \frac{1}{2} \|w\|^2 + \sum_{i=1}^{n} \lambda_i \left(1 - y_i(w^\top x_i + b)\right).$$

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Dual optimization problem:

$$\begin{aligned} \underset{\lambda \in \mathbb{R}^n}{\text{Maximize}} \quad & \phi(\lambda) := \textstyle\sum_{i=1}^{n} \lambda_i - \frac{1}{2}\left\|\sum_{i=1}^{n} \lambda_i y_i x_i\right\|^2 \\ \text{Subject to} \quad & \lambda \succeq \mathbf{0} \\ & \textstyle\sum_{i=1}^{n} \lambda_i y_i = 0 \end{aligned} \qquad \text{(Dual of Linear SVM)}$$

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Let (w^*, b^*) and λ^* be solutions to the (Linear SVM) and (Dual of Linear SVM), respectively.

KKT optimality conditions of linear SVM

$$
\begin{aligned}
1 - y_i(\langle w^*, x_i\rangle + b^*) &\leq 0\ , \quad i = 1, \ldots, n \\
\lambda^* &\succeq \mathbf{0} \\
\lambda_i^* \left(1 - y_i(\langle w^*, x_i\rangle + b^*)\right) &= 0\ , \quad i = 1, \ldots, n \\
w^* - \textstyle\sum_{i=1}^{n} \lambda_i^* y_i x_i &= \mathbf{0} \\
\textstyle\sum_{i=1}^{n} \lambda_i^* y_i &= 0
\end{aligned}
\tag{KKT Linear SVM}
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Support vectors: set of points (x_i, y_i) for which $\lambda_i^* > 0$. Due to complementary slackness, $y_i(\langle w^*, x_i\rangle + b) = 1$ (or $\langle w^*, x_i\rangle + b = y_i$) for all support vectors.

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$w^* = \sum_{i \in SV} \lambda_i^* y_i x_i$, where $SV \subseteq [n]$ denotes the index set of all the support vectors.

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For any $i \in SV$, $\langle w^*, x_i \rangle + b = y_i$. Thus, $b = y_i - \langle w^*, x_i \rangle = y_i - \sum_{j=1}^n \lambda_j^* y_j \langle x_j, x_i \rangle$.

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Exercise. Show that the largest margin of separation is equal to $\frac{1}{\sum_{i \in SV} \lambda_i^*}$.

Nonlinearly separable points

Suppose that the dataset $S = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ is NOT linearly separable. That is, the convex hulls of $S^+ = (x \mid (x, y) \in S\ ,\ \ y = +1)$ and $S^- = (x \mid (x, y) \in S\ ,\ \ y = -1)$ are NOT disjoint.

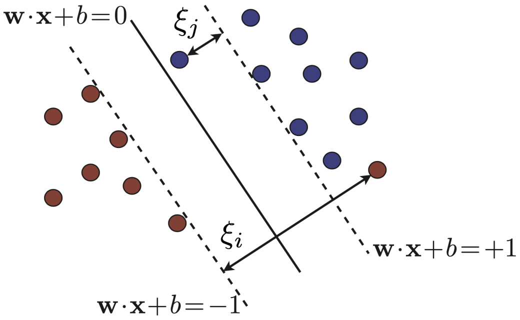

Figure: Nonlinearly separable points.

Linear SVM with soft margin

Slack variables. Introduce nonnegative variables $\xi_i, i = 1, \ldots, n$ such that for all i,

$$y_i(w^\intercal x_i + b) + \xi_i \geq 1$$

We call ξ_i's as *slack variables*.

Linear SVM with soft margin

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In this case, we train a linear SVM with **soft margin** using the following QP:

$$\begin{array}{cll} \underset{\xi \in \mathbb{R}^n,\ w \in \mathbb{R}^m,\ b \in \mathbb{R}}{\text{Minimize}} & \frac{1}{2}\left\|w\right\|^2 + \Psi(\xi_1, \ldots, \xi_n) & \\ \text{Subject to} & 1 - y_i(w^\intercal x_i + b) - \xi_i \leq 0 \quad , \ i = 1, \ldots, n & \\ & -\xi \preceq \mathbf{0} & \end{array} \qquad \text{(Soft-margin SVM)}$$

where, $\Psi(\xi_1, \ldots, \xi_n)$ is convex and typically taken to be $c \sum_{i=1}^n \xi_i^r$ for $r \geq 1$.

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We want ξ to be sparse. This can be approximately obtained by using $r = 1$.

Further readings

The lecture notes are based on Chapter 5 of "Foundations of Machine Learning" by M. Mohri, A. Rostamizadeh, and A. Talwalkar.

You may want to check out the following:

- **Learning guarantee of SVM:** Section 5.2.4 on *leave-one-out* (or *uniform stability*) analysis of SVM.
- **Generalizability of SVM:** Section 5.4 on *margin theory*.
- **Soft margin linear SVM:** More details can be found in Section 5.3.