Machine Learning and Neural Networks (MATH3431) Epiphany term, 2024

Handout 7: Support Vector Machines

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Aim. To introduce the Support Vector Machines as a procedure. Motivation, set-up, description, computation, and implementation. We focus on the classical treatment.

Reading list & references:

(1) Shalev-Shwartz, S., & Ben-David, S. (2014). Understanding machine learning: From theory to algorithms. Cambridge university press.
- Ch. 15 (pp. 167-170, 171-172, 176-177) Support Vector Machine

(2) Bishop, C. M. (2006). Pattern recognition and machine learning (Vol. 4, No. 4, p. 738). New York: Springer.
- Ch. 7.1 Sparse Kernel Machines/Maximum marginal classifiers

(3) Vapnik, V. (2013). The nature of statistical learning theory. Springer science & business media.

(4) Boyd, S. P., & Vandenberghe, L. (2004). Convex optimization. Cambridge university press.
- Ch. 4, 5

(5) Strang, G. (2019). Linear algebra and learning from data. Wellesley-Cambridge Press.

1. Intro and motivation

Note 1. Support Vector Machines (SVM) is a ML procedure for learning linear predictors in high-dimensional feature spaces with regards the sample complexity challenges. Due to a duality property, SVM have sparse solutions, so that predictions for new inputs depend only on quantities evaluated at a subset of the whole training dataset.

Definition 2. Let $w \neq 0$. **Hyperplane** in space $\mathcal{X} \subseteq \mathbb{R}^d$ is called the sub-set

$$S = \left\{ x \in \mathbb{R}^d : \langle w, x \rangle + b = 0 \right\}. \tag{1.1}$$

Note 3. Hyperplane (1.1) separates $\mathcal{X}$ in two half-spaces

$$S_+ = \left\{ x \in \mathbb{R}^d : \langle w, x \rangle + b > 0 \right\}$$

and

$$S_- = \left\{ x \in \mathbb{R}^d : \langle w, x \rangle + b < 0 \right\}$$

Definition 4. Halfspace (hypothesis space) is hypotheses class $\mathcal{H}$ designed for binary classification problems, $\mathcal{X} \subseteq \mathbb{R}^d$ and $\mathcal{Y} = \{-1, +1\}$ defined as

$$\mathcal{H} = \left\{ x \longmapsto \text{sign}\left(\langle w, x \rangle + b\right) : w \in \mathbb{R}^d, b \in \mathbb{R} \right\},$$

where b is called bias.

Definition 5. Each **halfspace hypothesis** $h \in \mathcal{H}$ has form

$$h_{w,b}(x) = \text{sign}(\langle w, x \rangle + b). \tag{1.2}$$

It takes an input in $\mathcal{X} \subseteq \mathbb{R}^d$ and returns an output in $\mathcal{Y} = \{-1, +1\}$. We may refer to it as halfspace (w, b) as well.

Note 6. Let $S = \{(x_i, y_i)\}_{i=1}^m$ be a training set of examples with $x_i \in \mathbb{R}^d$ the features and $y_i \in \{-1, +1\}$ the labels.

Note 7. Our goal is to train a halfspace hypothesis $h_{w,b}(x)$ in (1.2) against a training dataset S, with puppose to be able to classify a future feature x as $y = -1$ or $y = 1$.

Definition 8. The training set S is **linearly separable** if there exists a halfspace (w, b) such that for all $i = 1, ..., n$

$$y_i = \text{sign}(\langle w, x_i \rangle + b)$$

or equivalently

$$y_i(\langle w, x_i \rangle + b) > 0 \tag{1.3}$$

Note 9. Halfspaces (w^*, b^*) satisfying the linearly separable condition (1.3) are ERM hypothesis under the $0-1$ loss function $\ell^{0-1}((w, b), z) = 1_{(y_i \neq \text{sign}(\langle w, x_i \rangle + b))}$ and Empirical Risk $R_S^{0-1}(w, b) = \frac{1}{m}\sum_{i=1}^m \ell((w, b), z_i) \geq 0$, i.e.

$$(w^*, b^*) = \arg\min_{w,b} \left(R_S^{0-1}(w, b)\right) = \arg\min_{w,b} \left(\frac{1}{m}\sum_{i=1}^m \ell^{0-1}((w, b), z_i)\right)$$

as $R_S^{0-1}(w^*, b^*) = 0$.

Definition 10. Margin of a hyperplane with respect to a training set is defined to be the minimal distance between a point in the training set and the hyperplane.

Note 11. There are several different halfspaces (w, b) satisfying (1.3) for the same linearly separable training dataset S; see Figure (1.1; left).

Note 12. The rational is that if a hyperplane has a large margin, then it will still separate the training set even if we slightly perturb each instance.

Note 13. There are several different halfspaces (w, b) satisfying (1.3) for the same linearly separable training dataset S; see Figure (1.1; left). In Figure (1.1; right) the margin γ is the distance from the hyperplane (solid line) to the closest points in either class (which touch the parallel dotted lines). Among the hyperplanes satisfying (1.3), a reasonable/desirable halfspace (w, b) is the one with the maximum margin γ; see Figure (1.1; right). The rational is that if a hyperplane has a large margin, then it will still separate the training set even if we slightly perturb each instance.

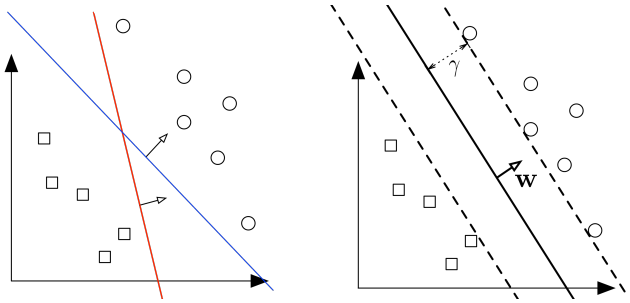


FIGURE 1.1

Note 14. Support Vector Machines (SVM) aims at learning the maximum margin separating hyperplane Figure (1.1; Right).

2. Hard Support Vector Machine

Assumption 15. *Assume the training sample* $S = \{(x_i, y_i)\}_{i=1}^m$ *is linearly separable.*

Definition 16. Hard Support Vector Machine (Hard-SVM) is the learning rule in which we return an ERM hyperplane that separates the training set with the largest possible margin given Assumption 15.

Problem 17. (Hard-SVM) Given a linearly separable training sample $S = \{(x_i, y_i)\}_{i=1}^m$ the Hard-SVM rule for the binary classification problem is the solution to the quadratic optimization problem:

Solve

$$\left(\tilde{w}, \tilde{b}\right) = \arg\min_{(w,b)} \frac{1}{2} \|w\|_2^2 \tag{2.1}$$

$$\text{subject to: } y_i \left(\langle w, x_i \rangle + b\right) \geq 1, \ \forall i = 1, ..., m \tag{2.2}$$

Scale

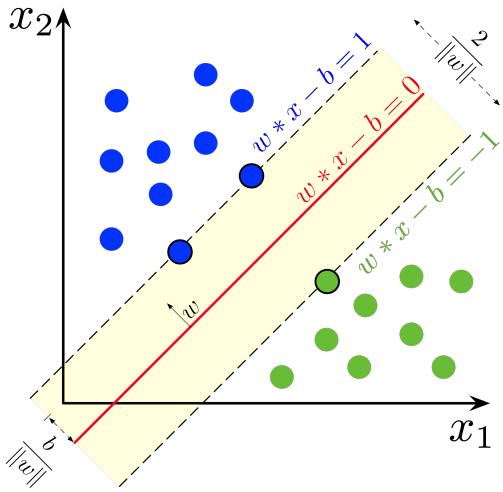
$$\hat{w} = \frac{\tilde{w}}{\|\tilde{w}\|}, \text{ and } \hat{b} = \frac{\tilde{b}}{\|\tilde{w}\|}$$

Note 18. Following we show why Problem 17 produces a Hard-SVM hyperplane stated in Note 16.

Proposition 19. *The distance between a point* x *and the hyperplane defined by* (w, b) *with is* $|\langle w, x \rangle + b| \,/\, \|w\|$.

Proof. We skip it. □

Note 20. On the right, see the geometry of Problem 17.



Note 21. Hard-SVM selects two parallel hyperplanes that separate the two classes of data so that the distance between them is as large as possible. The predictive hyperplane (rule) is the hyperplane that lies halfway between them.

Note 22. Hard-SVM in Problem 17 searches for the hyperplane with minimum norm w among all those that separate the data and have distance greater or equal to 1.

Proof. (Sketch of the proof of Problem 17)

(1) Based on Note 16, and Proposition 19, the closest point in the training set to the separating hyperplane has distance

$$\min_i \left(|\langle w, x_i \rangle + b| \,/\, \|w\| \right) \tag{2.3}$$

Without loss of generality, we make 2.3 identifiable by just pick those with $\|w\| = 1$. Hence, by Definition 16, the Hard-SVM hypothesis should be such as

$$(w^*, b^*) = \underset{(w,b):\|w\|=1}{\arg\max} \left(\min_i \left(|\langle w, x_i \rangle + b| \right) \right) \tag{2.4}$$

$$\text{subject to } \; y_i \left(\langle w, x_i \rangle + b \right) > 0, \; \forall i = 1, ..., m \tag{2.5}$$

(2) If there is a solution in (2.4) (namely, linearly separable dataset), then (2.4) is equivalent to (proof is omitted)

$$(w^*, b^*) = \underset{(w,b):\|w\|=1}{\arg\max} \left(\min_i \left(y_i \left(\langle w, x_i \rangle + b \right) \right) \right) \tag{2.6}$$

(3) Next we show that (2.6) is equivalent to the solution of Problem 17; i.e. $(w^*, b^*) = \left(\hat{w}, \hat{b} \right)$.
Let $\gamma^* := \min_i \left(|\langle w^*, x_i \rangle + b^*| \right)$. Firstly, because

$$y_i \left(\langle w^*, x_i \rangle + b^* \right) \geq \gamma^* \;\; \Leftrightarrow \;\; y_i \left(\langle \frac{w^*}{\gamma^*}, x_i \rangle + \frac{b^*}{\gamma^*} \right) \geq 1$$

$\left(\frac{w^*}{\gamma^*}, \frac{b^*}{\gamma^*} \right)$ satisfies condition (2.2). Secondly, I have $\|\tilde{w}\| \leq \left\| \frac{w^*}{\gamma^*} \right\| = \frac{1}{\gamma^*}$ because of (2.1) and because of $\|w^*\| = 1$. Hence, for all $i = 1, ..., m$, it is

$$y_i \left(\langle \hat{w}, x_i \rangle + \hat{b} \right) = \frac{1}{\|\tilde{w}\|} y_i \left(\langle \tilde{w}, x_i \rangle + \tilde{b} \right) \geq \frac{1}{\|\tilde{w}\|} \geq \gamma^*$$

Hence $\left(\hat{w}, \hat{b} \right)$ is the optimal solution of (2.6).

□

Definition 23. Homogeneous halfspaces in SVM is the case where the halfspaces pass from the origin; that is when the bias term in (2.2) is zero $b = 0$.

3. Soft Support Vector Machine

Note 24. Hard-SVM assumes the strong Assumption 15 that the training set is linearly separable. This might not always the case, and hence there is need to derive a procedure that weakens this assumption.

Note 25. Soft Support Vector Machine (Soft-SVM) aims to relax the strong assumption of Hard-SVM that the training set is linearly separable (2.5) with purpose to extend the scope of application. Soft-SVM does not assume Assumption 15. Soft-SVM rule is given as the solution to the quadratic optimization problem 26.

Problem 26. (Soft-SVM) Given a training sample $S = \{(x_i, y_i)\}_{i=1}^m$ the Soft-SVM rule for the binary classification learning problem is solution to the quadratic optimization problem

Solve

$$(w^*, b^*, \xi^*) = \underset{(w,b,\xi)}{\arg\min} \left(\frac{1}{2} \|w\|_2^2 + C \frac{1}{m} \sum_{i=1}^m \xi_i \right) \tag{3.1}$$

$$\text{subject to: } y_i \left(\langle w, x_i \rangle + b \right) \geq 1 - \xi_i, \ \forall i = 1, ..., m \tag{3.2}$$

$$\xi_i \geq 0, \ \forall i = 1, ..., m \tag{3.3}$$

Note 27. To relax the linearly separable training set Assumption 15, Soft-SVM relies on replacing the "harder" constraint (2.2) with the "softer" one in (3.2) through the introduction of non-negative unknown quantities (slack variables) $\{\xi_i\}_{i=1}^m$ controlling how much the separability assumption (2.2) is violated. Because any point that is misclassified has $\xi_i > 1$, it follows that $\sum_{i=1}^m \xi_i$ is an upper bound on the number of misclassified points.

Note 28. Parameter $C > 0$ controls the trade-off between the slack variable penalty and the margin. It controls the trade-off between minimizing training errors and controlling model complexity.

Note 29. Soft-SVM learns all (w, b, ξ) via the minimization part in (3.1) where the trade off between the two terms is controlled via the user specified parameter C.

Note 30. Proposition 31 shows that the Soft-SVM is a binary classification learning problem under the hinge loss function and with a regularization term biasing toward low norm separators.

Proposition 31. *The solution of Problem 26 is equivalent to the Ridge regularized loss minimization problem*

$$(w^*, b^*) = \underset{(w,b)}{\arg\min} \left(R_S^{hinge} + \lambda \|w\|_2^2 \right) \tag{3.4}$$

corresponding to a learning problem under the hinge loss function

$$\ell^{hinge} \left((w, b), z \right) = \max \left(0, 1 - y \left(\langle w, x \rangle + b \right) \right)$$

and hence the hinge Empirical Risk Function

$$R_S^{hinge}\left((w,b)\right) = \frac{1}{m}\sum_{i=1}^{m}\max\left(0, 1 - y_i\left(\langle w, x_i\rangle + b\right)\right)$$

regularization parameter $\lambda = \frac{1}{2C}$ *and regularization term* $\|\cdot\|_2^2$.

Proof. In Algorithm 26, we consider (3.1) as

$$\arg\min_{(w,b)}\left(\min_{\xi}\left(\lambda\|w\|_2^2 + \frac{1}{m}\sum_{i=1}^{m}\xi_i\right)\right) \tag{3.5}$$

with $\lambda = \frac{1}{2C}$. Consider (w,b) fixed and focus on the inside minimization. From (3.2), it is $\xi_i \geq 1 - y_i\left(\langle w^*, x_i\rangle + b^*\right)$, and from (3.3), it is $\xi_i \geq 0$. If $y_i\left(\langle w, x_i\rangle + b\right) \geq 1$, the best assignment in 3.5 is $\xi_i = 0$ because it is $\xi_i \geq 0$ from (3.3) and I need to minimize (3.5) wrt ξ_i's. If $y_i\left(\langle w, x_i\rangle + b\right) \leq 1$, the best assignment in (3.5) is $\xi_i = 1 - y_i\left(\langle w, x_i\rangle + b\right)$ because I need to minimize w.r.t ξ_i's. Hence $\xi_i = \max\left(0, 1 - y_i\left(\langle w, x_i\rangle + b\right)\right)$. □

Example 32. Consider the Soft-SVM as a Ridge regularized loss minimization problem in (3.4) on a training dataset $S = \{(x_i, y_i)\}_{i=1}^m$ with $z_i = (x_i, y_i) \overset{\text{ind}}{\sim} g$ where g is a data generating process on $\mathcal{X} \times \{0,1\}$ with $\mathcal{X} = \{x : \|x\| \leq \rho\}$. Let $\mathfrak{A}(S)$ be the solution of the Soft-SVM. Then:

- Because $\ell^{\text{hinge}}\left((w,b), z\right) = \max\left(0, 1 - y\left(\langle w, x\rangle + b\right)\right)$ is $\|x\|$-Lipschitz, it is

  $$\mathrm{E}_{S\sim g}\left(R_g^{\text{hinge}}\left(\mathfrak{A}(S)\right)\right) \leq R_g^{\text{hinge}}(u) + \lambda\|u\|^2 + \frac{2\rho^2}{\lambda m}$$

  [Hint: Note 43 Handout 3: Learnability and stability in learning problems]
- If we assume a bounded learning problem, i.e. $\mathcal{H} = \{\|(w,b)\| \leq B\}$ for $B > 0$ then

  $$\mathrm{E}_{S\sim g}\left(R_g^{\text{hinge}}\left(\mathfrak{A}(S)\right)\right) \leq \min_{\|(w,b)\|\leq B} R_g^{\text{hinge}}\left((w,b)\right) + \lambda B^2 + \frac{2\rho^2}{\lambda m}$$

- If we choose $\lambda = \sqrt{\frac{2\rho^2}{B^2 m}}$ then

  $$\mathrm{E}_{S\sim g}\left(R_g^{\text{hinge}}\left(\mathfrak{A}(S)\right)\right) \leq \min_{\|(w,b)\|\leq B} R_g^{\text{hinge}}\left((w,b)\right) + \sqrt{\frac{8\rho^2 B^2}{m}}$$

- Assume one was interested in minimizing a $0-1$ Risk $R_g^{0-1}(\cdot)$ under the $0-1$ loss $\ell^{0-1}\left((w,b), z\right) := 1_{(y\langle w,x\rangle \leq 0)}$. But $\ell^{0-1}(\cdot, z)$ is non-convex for all z. It is $\ell^{0-1}\left((w,b), z\right) \leq \ell^{\text{hinge}}\left((w,b), z\right)$ for all z. By using the convex hinge loss ℓ^{hinge} as a surrogate loss and implementing the Soft-SVM procedure, the error under $0-1$ Risk $R_g^{0-1}(\cdot)$ is

  $$\mathrm{E}_{S\sim g}\left(R_g^{0-1}\left(\mathfrak{A}(S)\right)\right) \leq \mathrm{E}_{S\sim g}\left(R_g^{\text{hinge}}\left(\mathfrak{A}(S)\right)\right) \leq \min_{\|(w,b)\|\leq B} R_g^{\text{hinge}}\left((w,b)\right) + \sqrt{\frac{8\rho^2 B^2}{m}}$$

Example 33. Given Proposition 31, Soft-SVM in Problem 26 can be learned via any variation of SGD, eg online SGD (batch size $m = 1$) with recursion

$$\varpi^{(t+1)} = \varpi^{(t)} - \eta_t v_t$$

$$\begin{bmatrix} w^{(t+1)} \\ b^{(t+1)} \end{bmatrix} = \begin{bmatrix} w^{(t)} \\ b^{(t)} \end{bmatrix} - \eta_t \begin{bmatrix} v_{w,t} \\ v_{b,t} \end{bmatrix}$$

where $v_{w,t} = \begin{cases} -y_i^{(t)} x_i^{(t)} & \text{if } y_i^{(t)} \left(\langle w^{(t)}, x_i^{(t)} \rangle + b^{(t)} \right) < 1 \\ 0 & \text{otherwise} \end{cases}$ and $v_{b,t} = \begin{cases} -y_i^{(t)} & \text{if } y_i^{(t)} \left(\langle w^{(t)}, x_i^{(t)} \rangle + b^{(t)} \right) < 1 \\ 0 & \text{otherwise} \end{cases}$.

4. Duality and sparsity

4.1. **Lagrangian duality .** Ref [4]

Notation 34. Let $f : \mathbb{R}^q \to \mathbb{R}$ be an objective function, let $\{g_i : \mathbb{R}^q \to \mathbb{R}\}_{i=1}^m$ inequality constraint convex functions, and let $\{h_j : \mathbb{R}^q \to \mathbb{R}\}_{j=1}^n$ equality constraint functions.

Definition 35. (Primal problem) Consider we have the following minimization problem that we will call Primal problem

$$\begin{aligned} p^* = \min_x \left(f(x) \right) \\ \text{s.t.} g_i(x) \leq 0, \ \ \forall i = 1, ..., m \\ h_j(x) = 0, \ \ \forall j = 1, ..., n \end{aligned} \tag{4.1}$$

Definition 36. (Lagrangian function) To the Primal problem 35, we associate the Lagrangian function $L : \mathbb{R}^q \times \mathbb{R}^m \times \mathbb{R}^n$ with

$$L(x, \alpha, \beta) = f(x) + \sum_{i=1}^m \alpha_i g_i(x) + \sum_{j=1}^n \beta_j h_j(x) \tag{4.2}$$

Note 37. Note that the Primal problem is equivalent to

$$p^* = \min_x \left(\max_{\alpha \geq 0, \beta} \left(L(x, \alpha, \beta) \right) \right)$$

For instance, if I ignore the $\{h_j\}$ terms which is zero for a suitable solution for simplicity, I observe that

$$\max_{\alpha \geq 0, \beta} \left(L(x, \alpha, \beta) \right) = \begin{cases} f(x) & g_i(x) \leq 0, \forall i \\ \infty, & g_i(x) > 0, \exists i \end{cases}$$

Definition 38. (Lagrangian dual problem) The associated Lagrangian dual problem is

$$\begin{aligned} d^* = \max_{\alpha, \beta} \left(\min_x \left(L(x, \alpha, \beta) \right) \right) \\ \text{s.t.} \alpha_i \geq 0 \\ \beta_j \in \mathbb{R} \end{aligned}$$

Definition 39. (Dual function) To the Dual problem, we associate a function $\tilde{L} : \mathbb{R}^m \times \mathbb{R}^n$ with

$$\tilde{L}(\alpha, \beta) := \min_x \left(L(x, \alpha, \beta) \right)$$

called dual function.

Proposition 40. *In general it is $p^* \geq d^*$; i.e.*

$$\min_x \max_{\alpha \geq 0, \beta} \left(L\left(x, \alpha, \beta\right)\right) \geq \max_{\alpha \geq 0, \beta} \min_x \left(L\left(x, \alpha, \beta\right)\right)$$

Definition 41. We call the general case $p^* \geq d^*$ weak duality.

Definition 42. When $p^* = d^*$ we say we have a strong duality.

Proposition 43. *(Strong duality via Slater condition) If the primal problem (4.1) is convex, and satisfies the weak Slater's condition, i.e.*

$$\left(\exists x_0 \in \mathcal{D}\right) \ : \ \left(g_i\left(x_0\right) < 0, \ \ \forall i = 1, ..., n\right) \text{ and } \left(h_i\left(x_0\right) = 0, \ \ \forall i = 1, ..., n\right)$$

then strong duality holds, that is: $p^* = d^*$. It other words

$$\min_x \max_{\alpha \geq 0, \beta} \left(L\left(x, \alpha, \beta\right)\right) = \max_{\alpha \geq 0, \beta} \min_x \left(L\left(x, \alpha, \beta\right)\right)$$

Proposition 44. *When f, $\{h_j\}$, $\{g_i\}$ are convex and the Slater condition holds, Karush–Kuhn–Tucker (KKT) conditions are necessary and sufficient conditions for x^* to be local minimum*

$$\begin{aligned}
0 =& \nabla f\left(x^*\right) + \sum_{j=1}^{n} \beta_j \nabla h_j\left(x^*\right) + \sum_{i=1}^{m} \alpha_i \nabla g_i\left(x^*\right) && \textit{Stationarity} \\
& g_i\left(x^*\right) \leq 0, \ \ \forall i = 1, ..., m && \textit{Primal feasibility} \\
& h_j\left(x^*\right) = 0, \ \ \forall j = 1, ..., n && \\
& \alpha_i \geq 0 \ \ \forall i = 1, ..., m && \textit{Dual feasibility} \\
& \alpha_i g_i\left(x^*\right) = 0, \ \ \forall i = 1, ..., m && \textit{Complementary slackness}
\end{aligned} \tag{4.3}$$

4.2. **Implementation in the Hand SVM.**

Note 45. The Hard-SVM Problem 17 (2.2) and (2.2), can be rewritten in the form

$$\min_w \left(\frac{1}{2} \left\| w \right\|_2^2 + g\left(w\right) \right) \tag{4.4}$$

with

$$g\left(w\right) = \max_{\alpha \geq 0} \sum_{i=1}^{m} \alpha_i \left(1 - y_i \left(\left\langle w, x_i \right\rangle + b \right)\right) = \begin{cases} 0 & \text{if } \ y_i \left(\left\langle w, x_i \right\rangle + b \right) \geq 1 \\ \infty & \text{else} \end{cases}$$

Hence we get the weak duality

$$\begin{aligned}
& \min_{w,b} \max_{\alpha \geq 0} \left(\frac{1}{2} \left\| w \right\|_2^2 + \sum_{i=1}^{m} \alpha_i \left(1 - y_i \left(\left\langle w, x_i \right\rangle + b \right)\right) \right) \\
& \geq \max_{\alpha \geq 0} \min_{w,b} \left(\underbrace{\frac{1}{2} \left\| w \right\|_2^2 + \sum_{i=1}^{m} \alpha_i \left(1 - y_i \left(\left\langle w, x_i \right\rangle + b \right)\right)}_{= L(w,b;\alpha)} \right)
\end{aligned} \tag{4.5}$$

Strong duality (equality) holds because of the convexity. Here, keeping α fixed, $L(w,\alpha,b)$ is minimized when

$$0 = \nabla_w L(w,\alpha,b)\big|_{(w^*,b^*)} \implies w^* = \sum_{i=1}^m \alpha_i y_i x_i \tag{4.6}$$

$$0 = \nabla_b L(w,\alpha,b)\big|_{(w^*,b^*)} \implies 0 = \sum_{i=1}^m \alpha_i y_i \tag{4.7}$$

The dual function is

$$\begin{aligned}\tilde{L}(\alpha) = \min_{w,b}(L(w,\alpha,b)) &= \frac{1}{2}\left\|\sum_{i=1}^m \alpha_i y_i x_i\right\|_2^2 - \sum_{i=1}^m \alpha_i \left(y_i\left(\langle\sum_{j=1}^m \alpha_j y_j x_j, x_i\rangle + b\right) - 1\right)\\ &= \sum_{i=1}^m \alpha_i - \frac{1}{2}\sum_{i=1}^m\sum_{j=1}^m \alpha_i\alpha_j y_i y_j \langle x_j x_i\rangle\end{aligned}$$

Then dual problem is

$$\max_{\alpha\in\mathbb{R}^m:\alpha\geq 0}\left(\sum_{i=1}^m \alpha_i - \frac{1}{2}\sum_{i=1}^m\sum_{j=1}^m \alpha_i\alpha_j y_i y_j \langle x_j x_i\rangle\right)$$

Note 46. The Dual problem of the Hard-SVM (primal) problem 17 is

$$\alpha^* = \arg\max_{\alpha\in\mathbb{R}^m:\alpha\geq 0}\left(\sum_{i=1}^m \alpha_i - \frac{1}{2}\sum_{i=1}^m\sum_{j=1}^m \alpha_i\alpha_j y_i y_j \langle x_j, x_i\rangle\right) \tag{4.8}$$

$$\text{subject to } 0 = \sum_{i=1}^m \alpha_i y_i$$

Note 47. Once the optimal α^* is computed from (4.8), the optimal weights w^* can be computed (from (4.6)) as

$$w^* = \sum_{i=1}^m \alpha_i^* y_i x_i \tag{4.9}$$

Note 48. If $\alpha_i^* = 0$, the example (x_i, y_i) does not contribute to (4.9). If $\alpha_i^* \neq 0$, (x_i, y_i) contributes to (4.9). Moreover if $\alpha_i^* \neq 0$ the KKT condition (4.3)

$$\alpha_i^*\left(y_i\left(\langle w^*, x_i\rangle + b^*\right) - 1\right) = 0$$

implies that $y_i\left(\langle w^*, x_i\rangle + b^*\right) = 1$ meaning that x_i is on the boundary of the margin. Features x_i associated to $\alpha_i^* \neq 0$ which contribute to the evaluation of the optimal weights w^* and hence the evaluation of the separating predictive rule $h_{w,b}$ are called **supporting vectors** (see Figure 4.1).

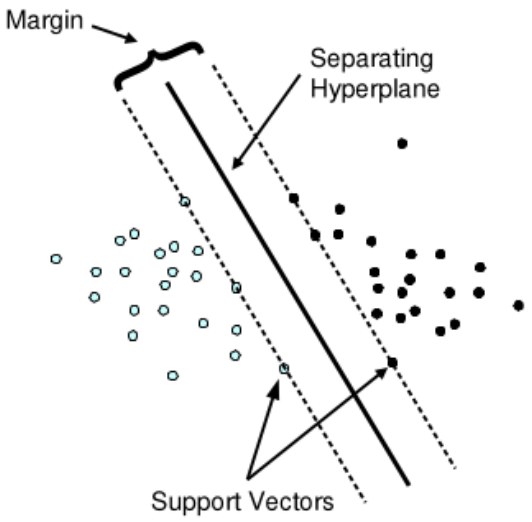


FIGURE 4.1

Note 49. Given optimal α^* (4.9) becomes

$$w^* = \sum_{i \in \mathcal{I}} \alpha_i^* y_i x_i \tag{4.10}$$

where $\mathcal{I} = \{i : y_i (\langle w^*, x_i \rangle + b^*) - 1 = 0\}$.

Note 50. The bias b parameter can be computed by KKT condition (4.3), it is

$$\alpha_i^* (y_i (\langle w^*, x_i \rangle + b^*) - 1) = 0$$

Consider $\mathcal{I} = \{i : y_i (\langle w^*, x_i \rangle + b^*) - 1 = 0\}$ then, for $i \in \mathcal{I}$ it is

$$y_i^2 (\langle w^*, x_i \rangle + b^*) - y_i = 0 \overset{y_i^2=1}{\Longrightarrow} \langle w^*, x_i \rangle + b^* - y_i = 0$$

and summing up all $i \in \mathcal{I}$, I get

$$\sum_{i \in \mathcal{I}} (\langle w^*, x_i \rangle + b^* - y_i) = 0 \implies b^* = \frac{1}{|\mathcal{I}|} \sum_{i \in \mathcal{I}} (y_i - \langle w^*, x_i \rangle) \tag{4.11}$$

Note 51. Therefore the predictive halfspace hypothesis is given as

$$\begin{aligned} h_{w,b}(x) &= \operatorname{sign} (\langle w^*, x \rangle + b^*) \\ &= \operatorname{sign} \left(\sum_{i \in \mathcal{I}} \alpha_i^* y_i \langle x_i, x \rangle + b^* \right) \end{aligned} \tag{4.12}$$

with $\mathcal{I} = \{i : y_i (\langle w^*, x_i \rangle + b^*) - 1 = 0\}$.

Note 52. Compared to the Primal problem (Problem 17), the dual problem (Note 46) is computationally desirable in cases that the training data size m is smaller than the number of the dimensions d of the feature space; i.e. $d \gg m$. The solution of the Primal quadratic programming problem in $d+1$ and complexity $O(d+1)$, while the dual quadratic programming problem has m variables and complexity $O(m)$.

Note 53. Compared to the Primal problem, the dual problem (Note 46), can provide sparse solutions relying on a small number of support vectors (see Eq. 4.10, 4.11, and 4.12).

Note 54. (Snapshot of the next concept "The kernel trick") The importance of the existence of the dual problem is that eg (4.8) and (4.12) involves the inner products between instances and does not require the direct access to specific elements of features within instance. For instance, if we consider the hypothesis (1.2) as an expansion of bases $h_{w,b}(x) = \text{sign}(\langle w, \phi(x)\rangle + b)$ with $\phi(x) = (\phi_1(x), ..., \phi_d(x))$ with a large d such as $d \gg m$ then, based on (4.12), the separation rule is

$$h_{w,b}(x) = \text{sign}\left(\sum_{i=1}^{m} \alpha_i y_i k(x_i, x) + b\right)$$

and 4.8 becomes

$$\alpha^* = \arg \max_{\alpha \in \mathbb{R}^m : \alpha \geq 0} \left(\sum_{i=1}^{m} \alpha_i - \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j k(x_i, x_j)\right)$$

with $k(x', x) = \langle \phi(x'), \phi(x)\rangle$. As we will see in the "kernel methods" lecture, in specific case, one can specify the "kernel" function $k(\cdot, \cdot)$ (having with specific desirable properties) avoiding the direct specification of a possibly high-dimensional dictionary of features $\{\phi_j(\cdot)\}$.

Note 55. In the Soft-SVM case, the solution is the same as in the Hard-SVM (4.9) and (4.12), the only difference is that in the quadratic programming problem (4.8) it is subject to $\alpha_j \in [0, C]$ where $C = 1/2\lambda$, it is called "cost" and controls the cost of having the constraint violation by adding the $\xi_i' s$. (See Exercise **??** from the Exercise sheet).

Note 56. Sparsity and duality in Soft SVM can be seen in Exercise 15 in the Exercise sheet.

Note 57. Relevance Vector Machine (a version of Bayesian SVM) can be seen in Exercise 16 in the Exercise sheet.