EE6550 Machine Learning

Lecture Three – Support Vector Machines

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Binary Classification Problem

- $\mathscr{I} \subseteq \mathbb{R}^N$: the input space.
- $\mathscr{Y}' = \mathscr{Y} = \{-1, +1\}$: the output, label space with loss function $L(y', y) = 1_{y' \neq y}$.
- c: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- $\mathcal{H}$: the hypothesis set.
- $S = (\mathbf{x}_1, \ldots, \mathbf{x}_m)$: a sample of m items, drawn i.i.d. from the input space according to P, with labels $(c(\mathbf{x}_1), \ldots, c(\mathbf{x}_m))$.
- Problem: find a hypothesis (binary classifier) $h : \mathscr{I} \to \{-1, +1\}$ in $\mathcal{H}$ with small generalization error

$$R(h) = E[1_{h(\mathbf{x}) \neq c(\mathbf{x})}] = P(h(\mathbf{x}) \neq c(\mathbf{x})).$$

Linear Binary Classifiers

- Occam's razor principle: hypothesis sets with smaller complexity – e.g., smaller VC-dimension or Rademacher complexity– provide better learning guarantees, when everything else being equal.
- A natural hypothesis set with relatively small complexity is that of linear classifiers, or halfspaces (represented by their boundary hyperplanes), which can be defined as follows:

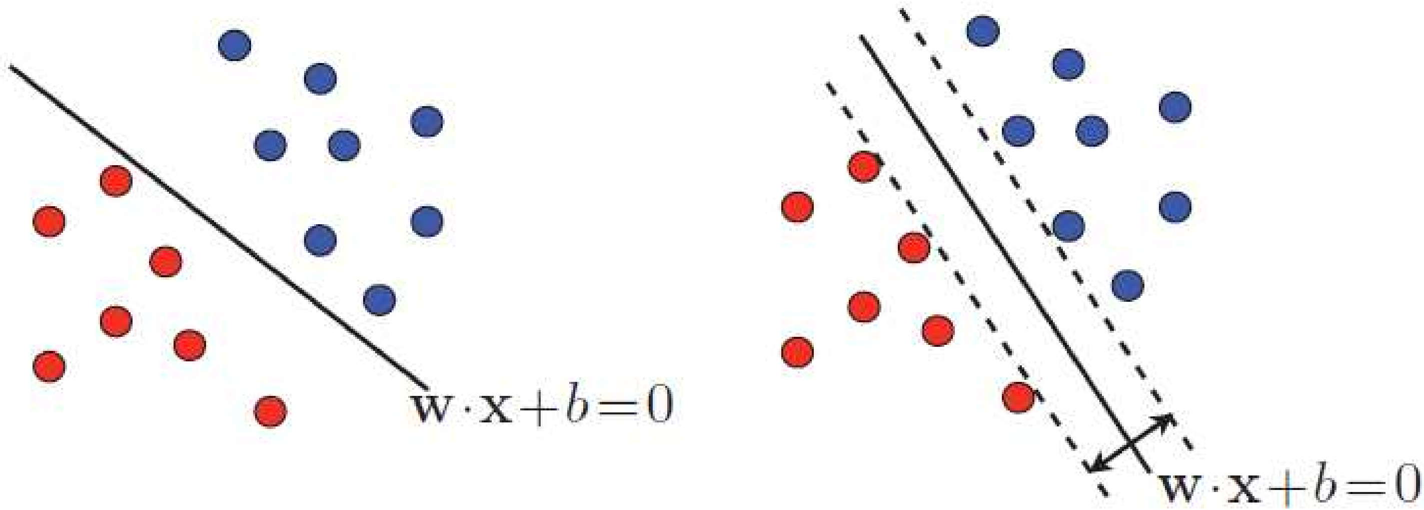
$$\mathcal{H} = \{\mathbf{x} \mapsto \mathrm{sgn}(\mathbf{w} \cdot \mathbf{x} + b) \mid \mathbf{w} \in \mathbb{R}^N,\ b \in \mathbb{R}\}.$$

The Contents of This Lecture

- Support vector machines - separable case.
- Support vector machines - general case.
- Margin guarantees.

Linearly Separable Labeled Training Samples

- $S = (\mathbf{x}_1, \ldots, \mathbf{x}_m)$: a labeled training sample of m items, drawn i.i.d. from the input space according to P, with labels $(c(\mathbf{x}_1), \ldots, c(\mathbf{x}_m))$.
- Assumption: there is a hyperplane $\mathbf{w} \cdot \mathbf{x} + b = 0$ which perfectly separates the training sample into two populations of positively and negatively labeled points.
- Existence of one perfectly separating hyperplane implies that of infinitely many such separating hyperplanes.
- Which hyperplane should a learning algorithm select?



Two possible separating hyperplanes.

SVM - Maximum-Margin Hyperplane

- $S = (\mathbf{x}_1, \ldots, \mathbf{x}_m)$: a linearly separable labeled training sample of m items, drawn i.i.d. from the input space according to P, with labels $(c(\mathbf{x}_1), \ldots, c(\mathbf{x}_m))$.
- $H : \mathbf{w} \cdot \mathbf{x} + b = 0$ with $c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b) > 0, 1 \leq i \leq m$: a perfectly separating hyperplane for S.
- Geometric margin of a perfectly separating hyperplane $(\mathbf{w}, b)$ with respective to S:

$$\rho = \min_{1 \leq i \leq m} \frac{|\mathbf{w} \cdot \mathbf{x}_i + b|}{\|\mathbf{w}\|}.$$

- The SVM algorithm will return a hyperplane with the maximum margin, or distance to the closest points, which is known as the maximum-margin hyperplane,

$$(\mathbf{w}, b)^{SVM} = \arg \max_{\substack{(\mathbf{w},b):c(\mathbf{x}_i)(\mathbf{w}\cdot\mathbf{x}_i+b)>0,1\leq i\leq m \\ \mathbf{w}\neq\mathbf{0}}} \min_{1\leq i\leq m} \frac{|\mathbf{w}\cdot\mathbf{x}_i + b|}{\|\mathbf{w}\|}.$$

Canonical Representation

The canonical representation of a perfectly separating hyperplane to a linearly separable labeled training sample $S = (\mathbf{x}_1, \ldots, \mathbf{x}_m)$ is an affine equation for the hyperplane

$$\mathbf{w} \cdot \mathbf{x} + b = 0$$

such that

$$\min_{1 \leq i \leq m} c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b) = 1.$$

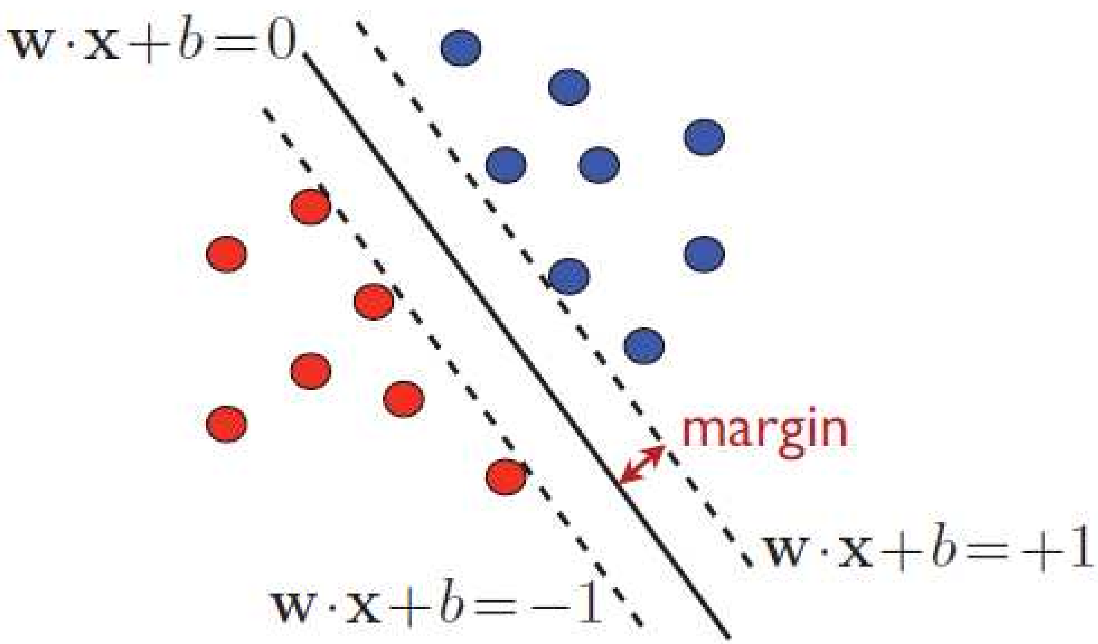
The geometric margin of a canonically represented perfectly separating hyperplane to S is

$$\rho = \min_{1 \leq i \leq m} \frac{|\mathbf{w} \cdot \mathbf{x}_i + b|}{\|\mathbf{w}\|} = \frac{1}{\|\mathbf{w}\|}.$$

- If a maximum-margin hyperplane is canonically represented as $\mathbf{w} \cdot \mathbf{x} + b = 0$, then the two hyperplanes

$$\mathbf{w} \cdot \mathbf{x} + b = \pm 1$$

are called marginal hyperplanes.



Margin Maximization Problem

$$
\begin{aligned}
\rho_{\max} &= \max_{\substack{(\mathbf{w},b):c(\mathbf{x}_i)(\mathbf{w}\cdot\mathbf{x}_i+b)>0,1\le i\le m\\ \mathbf{w}\neq\mathbf{0}}} \min_{1\le i\le m} \frac{|\mathbf{w}\cdot\mathbf{x}_i+b|}{\|\mathbf{w}\|}\\
&= \max_{\substack{(\mathbf{w},b):c(\mathbf{x}_i)(\mathbf{w}\cdot\mathbf{x}_i+b)>0,1\le i\le m\\ \mathbf{w}\neq\mathbf{0},\min_{1\le i\le m} c(\mathbf{x}_i)(\mathbf{w}\cdot\mathbf{x}_i+b)=1}} \min_{1\le i\le m} \frac{|\mathbf{w}\cdot\mathbf{x}_i+b|}{\|\mathbf{w}\|}\\
&\quad \text{by the scaling invariance of } (\mathbf{w},b)\\
&= \max_{\substack{(\mathbf{w},b):c(\mathbf{x}_i)(\mathbf{w}\cdot\mathbf{x}_i+b)>0,1\le i\le m\\ \mathbf{w}\neq\mathbf{0},\min_{1\le i\le m} c(\mathbf{x}_i)(\mathbf{w}\cdot\mathbf{x}_i+b)=1}} \frac{1}{\|\mathbf{w}\|}\\
&= \max_{\substack{(\mathbf{w},b):c(\mathbf{x}_i)(\mathbf{w}\cdot\mathbf{x}_i+b)\ge 1,1\le i\le m\\ \mathbf{w}\neq\mathbf{0}}} \frac{1}{\|\mathbf{w}\|} \text{ since at least one}\\
&\quad \text{inequality must reach the lower bound 1.}
\end{aligned}
$$

- Assumption: the sample S is not trivially labeled, i.e., the points in the sample S are neither all positively labeled nor all negatively labeled.

In this case, we have

$$\rho_{\max} = \max_{(\mathbf{w},b):c(\mathbf{x}_i)(\mathbf{w}\cdot\mathbf{x}_i+b)\geq 1, 1\leq i\leq m} \frac{1}{\|\mathbf{w}\|}.$$

The Primal Problem for SVM - Separable Case

$$
\begin{array}{ll}
\text{Minimize} & F(\mathbf{w}, b) = \frac{1}{2}\|\mathbf{w}\|^2 \\
\text{Subject to} & 1 - c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b) \leq 0, i = 1, \ldots, m \\
 & (\mathbf{w}, b) \in \mathbb{R}^N \times \mathbb{R}.
\end{array}
$$

- A quadratic programming (QP) problem.

Kuhn-Tucker Necessary Conditions for Local Minimal Solutions

Consider a nonlinear programming problem with equality constraints as well as inequality constraints, defined as

$$\begin{array}{ll} \text{Minimize} & f(\mathbf{x}) \\ \text{Subject to} & g_i(\mathbf{x}) \leq 0, i = 1, \ldots, m \\ & h_j(\mathbf{x}) = 0, j = 1, \ldots, l \\ & \mathbf{x} \in X, \end{array}$$

where X is a nonempty set in $\mathbb{R}^N$. Assume that

- $\bar{\mathbf{x}}$: a feasible solution, i.e., a point in X satisfying all equality constraints as well as inequality constraints;
- $I = \{i | g_i(\bar{\mathbf{x}}) = 0\}$;
- f and $g_i, i \in I$: differentiable at $\bar{\mathbf{x}}$;

- $g_i, i \notin I$: continuous at $\bar{\mathbf{x}}$;
- $h_j, j = 1, \ldots, l$: continuously differentiable at $\bar{\mathbf{x}}$;
- $\nabla g_i(\bar{\mathbf{x}})$ for $i \in I$ and $\nabla h_j(\bar{\mathbf{x}})$ for $j = 1, \ldots, l$ are linearly independent.

If $\bar{\mathbf{x}}$ is a local minimal solution, then there exist scalars λ_i for all $i \in I$ and μ_j for $j = 1, \ldots, l$ such that

$$\begin{aligned} \nabla f(\bar{\mathbf{x}}) + \sum_{i \in I} \lambda_i \nabla g_i(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \mu_j \nabla h_j(\bar{\mathbf{x}}) = \mathbf{0} \\ \lambda_i \ \geq \ 0 \text{ for all } i \in I \end{aligned}$$

In addition, if $g_i, i \notin I$, are also differentiable at $\bar{\mathbf{x}}$, then an equivalent form can be written as

$$\begin{aligned} \nabla f(\bar{\mathbf{x}}) + \sum_{i=1}^{m} \lambda_i \nabla g_i(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \mu_j \nabla h_j(\bar{\mathbf{x}}) = \mathbf{0} \\ \lambda_i g_i(\bar{\mathbf{x}}) = 0 \text{ for all } i = 1, \ldots, m \\ \lambda_i \ \geq \ 0 \text{ for all } i = 1, \ldots, m. \end{aligned}$$

- The scalars $\lambda_1, \dots \lambda_m$ and $\mu_1, \dots, \mu_l$ are called Lagrangian multipliers.
- The conditions $\lambda_i g_i(\bar{\mathbf{x}}) = 0$, $i = 1, \dots, m$, are called complementary slackness conditions.

Remark: If the feasible solution $\bar{\mathbf{x}}$ is a boundary point of X, the differentiability of f, g_i, and h_j at $\bar{\mathbf{x}}$ implicitly assumes that f, g_i, and h_j are defined in a neighborhood of $\bar{\mathbf{x}}$.

Various Convexity and Concavity Concepts

- $S \subseteq X$: the set of all feasible solutions of the nonlinear programming problem, called the feasible region, defined as

  $$S \triangleq \{\mathbf{x} \in X \mid g_i(\boldsymbol{x}) \leq 0, i = 1, \ldots, m, \text{ and } h_j(\boldsymbol{x}) = 0, j = 1, \ldots, l\}.$$

- A real-valued function u is said to be pseudoconvex at a feasible solution $\hat{\mathbf{x}}$ in S if it is differentiable at $\hat{\mathbf{x}}$ and $\nabla u(\hat{\mathbf{x}})^T(\mathbf{x} - \hat{\mathbf{x}}) \geq 0$ for $\mathbf{x} \in S$ implies that $u(\mathbf{x}) \geq u(\hat{\mathbf{x}})$.

- A real-valued function u is said to be pseudoconcave at a feasible solution $\hat{\mathbf{x}}$ in S if $-u$ is pseudoconvex at $\hat{\mathbf{x}}$.

- A real-valued function u is said to be quasiconvex at a feasible solution $\hat{\mathbf{x}}$ in S if u is defined in a convex set containing S and

  $$u(\lambda\mathbf{x} + (1 - \lambda)\hat{\mathbf{x}}) \leq \max\{u(\mathbf{x}), u(\hat{\mathbf{x}})\}$$

for all $\lambda \in (0,1)$ and all $\boldsymbol{x} \in S$.

- A real-valued function u is said to be quasiconcave at a feasible solution $\hat{\mathbf{x}}$ in S if $-u$ is quasiconvex at $\hat{\mathbf{x}}$.

- A real-valued function u is said to be convex at a feasible solution $\hat{\mathbf{x}}$ in S if u is defined in a convex set containing S and

$$u(\lambda\mathbf{x} + (1-\lambda)\hat{\mathbf{x}}) \leq \lambda u(\mathbf{x}) + (1-\lambda)u(\hat{\mathbf{x}})$$

  for all $\lambda \in (0,1)$ and all $\mathbf{x} \in S$.

- A real-valued function u is said to be concave at a feasible solution $\hat{\mathbf{x}}$ in S if $-u$ is convex at $\hat{\mathbf{x}}$.

- If a real-valued function u is both convex and differentiable at a feasible solution $\hat{\mathbf{x}}$ in S, then it is pseudoconvex at $\hat{\mathbf{x}}$.

- If a real-valued function u is convex at a feasible solution $\hat{\mathbf{x}} \in S$, then it is quasiconvex at $\hat{\mathbf{x}}$.

Kuhn-Tucker Sufficient Conditions for Global Minimum Solutions

Consider a nonlinear programming problem with inequality as well as equality constraints, defined as

$$\begin{aligned} \text{Minimize} \quad & f(\mathbf{x}) \\ \text{Subject to} \quad & g_i(\mathbf{x}) \leq 0, i = 1, \ldots, m \\ & h_j(\mathbf{x}) = 0, j = 1, \ldots, l \\ & \mathbf{x} \in X, \end{aligned}$$

where X is a nonempty set in $\mathbb{R}^N$. Assume that

- $\bar{\mathbf{x}}$: a feasible solution;
- $I = \{i | g_i(\bar{\mathbf{x}}) = 0\}$.

Assume that the Kuhn-Tucker necessary conditions hold true at $\bar{\mathbf{x}}$, i.e., there exist scalars $\lambda_i \geq 0, i \in I$, and $\mu_j \in \mathbb{R}, j = 1, 2, \ldots, l$, such that

$$\nabla f(\bar{\mathbf{x}}) + \sum_{i \in I} \lambda_i \nabla g_i(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \mu_j \nabla h_j(\bar{\mathbf{x}}) = \mathbf{0}.$$

In addition, if $g_i, i \notin I$, are also differentiable at $\bar{\mathbf{x}}$, then an equivalent form of the Kuhn-Tucker necessary conditions can be written as

$$\begin{aligned} \nabla f(\bar{\mathbf{x}}) + \textstyle\sum_{i=1}^{m} \lambda_i \nabla g_i(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \mu_j \nabla h_j(\bar{\mathbf{x}}) &= \mathbf{0} \\ \lambda_i g_i(\bar{\mathbf{x}}) = 0 \text{ for all } i &= 1, \ldots, m \\ \lambda_i \ \geq \ 0 \text{ for all } i &= 1, \ldots, m. \end{aligned}$$

Also assume that

- $J = \{j | \mu_j > 0\}$ and $K = \{j | \mu_j < 0\}$;
- f: pseudoconvex at $\bar{\mathbf{x}}$;
- $g_i, i \in I$: quasiconvex at $\bar{\mathbf{x}}$;

- $h_j, j \in J$: quasiconvex at $\bar{\mathbf{x}}$;
- $h_j, j \in K$: quasiconcave at $\bar{\mathbf{x}}$.

Then $\bar{\mathbf{x}}$ is a global minimum solution.

Convex Function

Let

- X: a nonempty open convex subset of $\mathbb{R}^n$;
- $f : X \to \mathbb{R}$: a twice differentiable function.

Then $f(\mathbf{x})$ is convex on X, i.e.,

$f(\lambda\mathbf{x}_1 + (1-\lambda)\mathbf{x}_2) \le \lambda f(\mathbf{x}_1) + (1-\lambda)f(\mathbf{x}_2)\ \forall\ \mathbf{x}_1, \mathbf{x}_2 \in X,\ \lambda \in (0,1)$

if and only if its Hessian matrix $\mathbf{H}(\mathbf{x})$ is positive semi-definite, i.e.,

$$\mathbf{v}^T\mathbf{H}(\mathbf{x})\mathbf{v} \ge 0,\ \forall\ \mathbf{v} \in \mathbb{R}^n,$$

for all $\mathbf{x} \in X$.

Qualification of the Primal Problem

- The object function $F(\mathbf{w}, b) = \frac{1}{2}\|\mathbf{w}\|^2$ is infinitely differentiable and convex so that it is pseudoconvex at any feasible point.
- The inequality constraint functions $g_i(\mathbf{w}, b) = 1 - c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b), 1 \leq i \leq m$, are affine functions so that they are infinitely differentiable and convex and then quasiconvex at any feasible point.
- $\nabla F = [\mathbf{w}^T 0]^T$, $\nabla g_i = -c(\mathbf{x}_i)[\mathbf{x}_i^T 1]^T$.
- The Kuhn-Tucker necessary conditions are:

$$\nabla F + \sum_{i=1}^m \lambda_i \nabla g_i = \mathbf{0} \Leftrightarrow \mathbf{w} = \sum_{i=1}^m \lambda_i c(\mathbf{x}_i)\mathbf{x}_i, 0 = \sum_{i=1}^m \lambda_i c(\mathbf{x}_i)$$

$$\lambda_i g_i(\mathbf{w}, b) = 0,\ i = 1, 2, \ldots, m$$

$$\lambda_i \geq 0,\ i = 1, 2, \ldots, m.$$

- Any feasible point $(\mathbf{w}, b)$ which satisfies the Kuhn-Tucker necessary conditions in above is a global minimum solution.
- The weight vector $\mathbf{w}$ solution of the SVM problem is a linear combination of the training set vectors $\mathbf{x}_1, \ldots, \mathbf{x}_m$.

Support Vectors

- Support vectors: any vector $\mathbf{x}_i$ which appears in the linear combination $\mathbf{w} = \sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i)\mathbf{x}_i$ with $\lambda_i \neq 0$.
- If $\lambda_i \neq 0$, we must have $c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b) = 1$ by the complementary slackness conditions.
- Support vectors lie in the two marginal hyperplanes $\mathbf{w} \cdot \mathbf{x} + b = \pm 1$.

Remarks

- Support vectors fully define the maximum-margin hyperplane or SVM solution.
- Vectors in the sample not lying on the marginal hyperplanes do not affect the solution to the SVM problem.
- While the solution $\mathbf{w}$ of the SVM problem is unique, the support vectors are not.

How to Determine Optimal Lagrangian Variables λ_i^{SVM} ?

- Once optimal Lagrangian variables λ_i^{SVM} are determined, we can compute

$$\mathbf{w}^{SVM} = \sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)\mathbf{x}_i$$

and for any support vector $\mathbf{x}_j$, we have

$$b^{SVM} = c(\mathbf{x}_j) - \mathbf{w}^{SVM} \cdot \mathbf{x}_j = c(\mathbf{x}_j) - \sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)(\mathbf{x}_i \cdot \mathbf{x}_j).$$

- We will use the Lagrangian dual problem to determine optimal λ_i^{SVM}.

The Existence and Uniqueness of the Solution for the Primal Problem for SVM - Separable Case

- The feasible region $S = \{(\mathbf{w}, b) \in \mathbb{R}^{N+1} \mid 1 - c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b) \leq 0, 1 \leq i \leq m\}$ is a nonempty polyhedra set in $\mathbb{R}^{N+1}$.
- The projection $\pi(S)$ of the polyhedra set S onto $\mathbb{R}^N$ by $\pi((\mathbf{w}, b)) = \mathbf{w}$ is a polyhedra set in $\mathbb{R}^N$.
- A polyhedra set is a closed convex set.
- Any nonempty closed convex set in $\mathbb{R}^N$ contains a unique element of smallest length.
- The unique element $\mathbf{w}^{SVM}$ in $\pi(S)$ of smallest length minimizes $\frac{1}{2}\|\mathbf{w}\|^2$ among all $\mathbf{w} \in \pi(S)$.
- The unique b^{SVM} is equal to $c(\mathbf{x}_j) - \mathbf{w}^{SVM} \cdot \mathbf{x}_j$ by any support vector $\mathbf{x}_j$.

Lagrangian Dual Function

- Primal problem:

$$
\begin{aligned}
\text{Minimize} \quad & f(\mathbf{x}) \\
\text{Subject to} \quad & g_i(\mathbf{x}) \leq 0, i = 1, \ldots, m \\
& h_j(\mathbf{x}) = 0, j = 1, \ldots, l \\
& \mathbf{x} \in X,
\end{aligned}
$$

  where X is a nonempty set in $\mathbb{R}^n$.

- Lagrangian function: for all $\mathbf{x} \in X$, $\lambda \in \mathbb{R}^m$, and $\nu \in \mathbb{R}^k$,

$$L(\mathbf{x}, \lambda, \nu) \triangleq f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{x}) + \sum_{j=1}^{k} \nu_j h_j(\mathbf{x}).$$

- Lagrangian dual function: for all $\lambda \in \mathbb{R}^m$ and $\nu \in \mathbb{R}^k$,

$$\theta(\lambda, \nu) \triangleq \inf_{\mathbf{x} \in X} L(\mathbf{x}, \lambda, \nu) = \inf_{\mathbf{x} \in X} \left(f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{x}) + \sum_{j=1}^{k} \nu_j h_j(\mathbf{x}) \right).$$

Global Minimum of a Convex Function

Let

- X: a nonempty open convex subset of $\mathbb{R}^n$;
- $f : X \to \mathbb{R}$: a differentiable convex function.

Then $\bar{\mathbf{x}}$ is an optimal solution to the minimization of $f(\mathbf{x})$ subject to $\mathbf{x} \in X$ if and only if $\nabla f(\bar{\mathbf{x}}) = \mathbf{0}$.

Lagrangian Dual Function for SVM - Separable Case

- $X = \mathbb{R}^N \times \mathbb{R}$: a nonempty open convex set.
- Lagrangian function: for all $\mathbf{w} \in \mathbb{R}^N, b \in \mathbb{R}$, and $\lambda \in \mathbb{R}^m$,

$$\begin{aligned} L(\mathbf{w}, b, \lambda) &= F(\mathbf{w}, b) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{w}, b) \\ &= \frac{1}{2}\|\mathbf{w}\|^2 + \sum_{i=1}^{m} \lambda_i (1 - c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b)) \end{aligned}$$

- For any fixed $\lambda \in \mathbb{R}^m$, the gradient ∇L of the Lagrangian function w.r.t. $(\mathbf{w}, b)$ is

$$\begin{aligned}
\nabla L &= \nabla F + \sum_{i=1}^{m} \lambda_i \nabla g_i \\
&= \begin{bmatrix} \mathbf{w} \\ 0 \end{bmatrix} - \sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i) \begin{bmatrix} \mathbf{x}_i \\ 1 \end{bmatrix}
\end{aligned}$$

and the Hessian matrix is

$$\mathbf{H} = \begin{bmatrix} I_{N \times N} & \mathbf{0} \\ \mathbf{0}^T & 0 \end{bmatrix}$$

which is positive semi-definite.

- For any fixed $\lambda \in \mathbb{R}^m$, the Lagrangian function is differentiable and convex over a non-empty open convex set X so that $(\hat{\mathbf{w}}, \hat{b})$ is an optimal solution to the minimization of $L(\mathbf{w}, b, \lambda)$ subject to $(\mathbf{w}, b) \in X$ if and only if $\nabla L(\hat{\mathbf{w}}, \hat{b}, \lambda) = \mathbf{0}$ if and only if

$$\hat{\mathbf{w}} = \sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i)\mathbf{x}_i \quad \text{and} \quad 0 = \sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i).$$

  – Note that for a fixed $\lambda \in \mathbb{R}^m$, $\sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i) \neq 0$ if and only if the infimum of the Lagrangian function $L(\mathbf{w}, b, \lambda)$ is $-\infty$.

- Lagrangian dual function: for all $\lambda \in \mathbb{R}^m$,

$$
\begin{aligned}
\theta(\lambda) &= \inf_{(\mathbf{w},b)\in X} L(\mathbf{w}, b, \lambda) \\
&= \begin{cases} \frac{1}{2}\|\hat{\mathbf{w}}\|^2 + \sum_{i=1}^m \lambda_i (1 - c(\mathbf{x}_i)(\hat{\mathbf{w}} \cdot \mathbf{x}_i + \hat{b})), \\ \qquad\qquad\qquad\qquad\qquad \text{if } \sum_{i=1}^m \lambda_i c(\mathbf{x}_i) = 0, \\ -\infty, \text{ if } \sum_{i=1}^m \lambda_i c(\mathbf{x}_i) \neq 0 \end{cases} \\
&= \begin{cases} \sum_{i=1}^m \lambda_i - \frac{1}{2} \sum_{i,j=1}^m \lambda_i \lambda_j c(\mathbf{x}_i) c(\mathbf{x}_j)(\mathbf{x}_i \cdot \mathbf{x}_j), \\ \qquad\qquad\qquad\qquad\qquad \text{if } \sum_{i=1}^m \lambda_i c(\mathbf{x}_i) = 0, \\ -\infty, \text{ if } \sum_{i=1}^m \lambda_i c(\mathbf{x}_i) \neq 0 \end{cases}
\end{aligned}
$$

Lagrangian Dual Problem

$$\begin{array}{ll} \text{Maximize} & \theta(\mathbf{u}, \mathbf{v}) \\ \text{Subject to} & u_i \geq 0, i = 1, \ldots, m \\ & \mathbf{u} \in \mathbb{R}^m, \mathbf{v} \in \mathbb{R}^k \end{array}$$

- Also referred to as the max-min dual problem.
- Given a primal problem, several Lagrangian dual problems can be devised, depending on which constraints are handled as $g_i(\mathbf{x}) \leq 0$ and $h_j(\mathbf{x}) = 0$ and which constraints are treated by the set X.

Lagrangian Dual Problem for SVM - Separable Case

$$
\begin{array}{ll}
\text{Maximize} & \theta(\lambda) = \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j c(\mathbf{x}_i) c(\mathbf{x}_j)(\mathbf{x}_i \cdot \mathbf{x}_j) \\
\text{Subject to} & \lambda_i \geq 0, i = 1, \ldots, m \\
& \sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i) = 0 \\
& \lambda \in \mathbb{R}^m
\end{array}
$$

- A quadratic programming (QP) problem.

Kuhn-Tucker Necessary Conditions for Local Maximal Solutions

Consider a nonlinear programming problem with equality constraints as well as inequality constraints, defined as

$$\begin{array}{ll} \text{Maximize} & f(\mathbf{x}) \\ \text{Subject to} & g_i(\mathbf{x}) \geq 0, i = 1, \ldots, m \\ & h_j(\mathbf{x}) = 0, j = 1, \ldots, l \\ & \mathbf{x} \in X, \end{array}$$

where X is a nonempty set in $\mathbb{R}^N$. Let

- $\bar{\mathbf{x}}$: a feasible solution, i.e., a point in X satisfying all equality constraints as well as inequality constraints;
- $I = \{i | g_i(\bar{\mathbf{x}}) = 0\}$;
- f and $g_i, i \in I$: differentiable at $\bar{\mathbf{x}}$;

- $g_i, i \notin I$: continuous at $\bar{\mathbf{x}}$;
- $h_j, j = 1, \ldots, l$: continuously differentiable at $\bar{\mathbf{x}}$;
- $\nabla g_i(\bar{\mathbf{x}})$ for $i \in I$ and $\nabla h_j(\bar{\mathbf{x}})$ for $j = 1, \ldots, l$ are linearly independent.

If $\bar{\mathbf{x}}$ is a local optimal solution, then there exist scalars λ_i for all $i \in I$ and μ_j for $j = 1, \ldots, l$ such that

$$\nabla f(\bar{\mathbf{x}}) + \sum_{i \in I} \lambda_i \nabla g_i(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \mu_j \nabla h_j(\bar{\mathbf{x}}) = \mathbf{0}$$
$$\lambda_i \;\geq\; 0 \text{ for all } i \in I$$

In addition, if $g_i, i \notin I$, are also differentiable at $\bar{\mathbf{x}}$, then an equivalent form can be written as

$$\nabla f(\bar{\mathbf{x}}) + \sum_{i=1}^{m} \lambda_i \nabla g_i(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \mu_j \nabla h_j(\bar{\mathbf{x}}) = \mathbf{0}$$
$$\lambda_i g_i(\bar{\mathbf{x}}) = 0 \text{ for all } i = 1, \ldots, m$$
$$\lambda_i \;\geq\; 0 \text{ for all } i = 1, \ldots, m.$$

Kuhn-Tucker Sufficient Conditions for Global Maximum Solutions

Consider a nonlinear programming problem with inequality as well as equality constraints, defined as

$$\begin{array}{ll} \text{Maximize} & f(\mathbf{x}) \\ \text{Subject to} & g_i(\mathbf{x}) \geq 0, i = 1, \ldots, m \\ & h_j(\mathbf{x}) = 0, j = 1, \ldots, l \\ & \mathbf{x} \in X, \end{array}$$

where X is a nonempty set in $\mathbb{R}^N$. Let

- $\bar{\mathbf{x}}$: a feasible solution;
- $I = \{i | g_i(\bar{\mathbf{x}}) = 0\}$.

Assume that the Kuhn-Tucker necessary conditions hold true at $\bar{\mathbf{x}}$, i.e., there exist scalars $\lambda_i \geq 0, i \in I$, and $\mu_j \in \mathbb{R}, j = 1, 2, \ldots, l$, such that

$$\nabla f(\bar{\mathbf{x}}) + \sum_{i \in I} \lambda_i \nabla g_i(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \mu_j \nabla h_j(\bar{\mathbf{x}}) = \mathbf{0}.$$

In addition, if $g_i, i \notin I$, are also differentiable at $\bar{\mathbf{x}}$, then an equivalent form of the Kuhn-Tucker necessary conditions can be written as

$$\begin{aligned} \nabla f(\bar{\mathbf{x}}) + \textstyle\sum_{i=1}^{m} \lambda_i \nabla g_i(\bar{\mathbf{x}}) + \sum_{j=1}^{l} \mu_j \nabla h_j(\bar{\mathbf{x}}) &= \mathbf{0} \\ \lambda_i g_i(\bar{\mathbf{x}}) = 0 \text{ for all } i &= 1, \ldots, m \\ \lambda_i \ \geq \ 0 \text{ for all } i &= 1, \ldots, m. \end{aligned}$$

Also assume that

- $J = \{j | \mu_j > 0\}$ and $K = \{j | \mu_j < 0\}$;
- f: pseudoconcave at $\bar{\mathbf{x}}$;
- $g_i, i \in I$: quasiconcave at $\bar{\mathbf{x}}$;

- $h_j, j \in J$: quasiconcave at $\bar{\mathbf{x}}$;
- $h_j, j \in K$: quasiconvex at $\bar{\mathbf{x}}$.

Then $\bar{\mathbf{x}}$ is a global maximum solution.

Concave Function

Let

- X: a nonempty open convex subset of $\mathbb{R}^n$;
- $f : X \to \mathbb{R}$: a twice differentiable function.

Then $f(\mathbf{x})$ is concave on X, i.e.,

$f(\lambda \mathbf{x}_1 + (1-\lambda)\mathbf{x}_2) \geq \lambda f(\mathbf{x}_1) + (1-\lambda) f(\mathbf{x}_2) \ \forall\ \mathbf{x}_1, \mathbf{x}_2 \in X,\ \lambda \in (0,1)$

if and only if its Hessian matrix $\mathbf{H}(\mathbf{x})$ is negative semi-definite, i.e.,

$$\mathbf{v}^T \mathbf{H}(\mathbf{x}) \mathbf{v} \leq 0,\ \forall\ \mathbf{v} \in \mathbb{R}^n,$$

for all $\mathbf{x} \in X$.

Qualification of the Dual Problem

- The object function

$$\theta(\lambda) = \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j c(\mathbf{x}_i) c(\mathbf{x}_j)(\mathbf{x}_i \cdot \mathbf{x}_j)$$

  is infinitely differentiable and concave so that it is pseudoconcave at any feasible point.

- The inequality constraint functions $g_i(\lambda) = \lambda_i, 1 \leq i \leq m$, and the equality constraint function $h(\lambda) = \sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i)$ are affine functions so that they are infinitely differentiable, concave and convex and then quasiconcave and quasiconvex at any feasible point.

- $\nabla\theta(\lambda) = \mathbf{1} - \mathbf{A}\lambda$, where $\mathbf{A}$ is the Gram matrix of the vectors $c(\mathbf{x}_i)\mathbf{x}_i, i = 1, 2, \ldots, m$,

$$
\begin{aligned}
&\mathbf{A} \\
= \;& [c(\mathbf{x}_i)\mathbf{x}_i \cdot c(\mathbf{x}_j)\mathbf{x}_j] \\
= \;& \begin{bmatrix}
c(\mathbf{x}_1)\mathbf{x}_1 \cdot c(\mathbf{x}_1)\mathbf{x}_1 & \cdots & c(\mathbf{x}_1)\mathbf{x}_1 \cdot c(\mathbf{x}_m)\mathbf{x}_m \\
c(\mathbf{x}_2)\mathbf{x}_2 \cdot c(\mathbf{x}_1)\mathbf{x}_1 & \cdots & c(\mathbf{x}_2)\mathbf{x}_2 \cdot c(\mathbf{x}_m)\mathbf{x}_m \\
\vdots & \ddots & \vdots \\
c(\mathbf{x}_m)\mathbf{x}_m \cdot c(\mathbf{x}_1)\mathbf{x}_1 & \cdots & c(\mathbf{x}_m)\mathbf{x}_m \cdot c(\mathbf{x}_m)\mathbf{x}_m
\end{bmatrix}
\end{aligned}
$$

- $\nabla g_i(\lambda) = \mathbf{e}_i, i = 1, 2, \ldots, m$, and $\nabla h(\lambda) = [c(\mathbf{x}_1), \ldots, c(\mathbf{x}_m)]^T$.

- The Kuhn-Tucker necessary conditions are:

$$\nabla\theta + \sum_{i=1}^{m} u_i \nabla g_i + v\nabla h = \mathbf{0} \Leftrightarrow \mathbf{A}\lambda = \mathbf{1} + \mathbf{u} + v \begin{bmatrix} c(\mathbf{x}_1) \\ \vdots \\ c(\mathbf{x}_m) \end{bmatrix}$$

$$u_i\lambda_i = 0,\ \ i = 1, 2, \ldots, m$$

$$u_i \geq 0,\ \ i = 1, 2, \ldots, m.$$

- Any feasible point λ which satisfies the Kuhn-Tucker necessary conditions in above is a global maximum solution.

Weak Duality Theorem

Assume that

- $\mathbf{x}$: a feasible solution to the primal problem P, i.e., $\mathbf{x} \in X, \mathbf{g}(\mathbf{x}) \leq \mathbf{0}, \mathbf{h}(\mathbf{x}) = \mathbf{0}$;
- $(\mathbf{u}, \mathbf{v})$: a feasible solution to the dual problem D, i.e., $\mathbf{u} \geq \mathbf{0}$.

Then we have

$$f(\mathbf{x}) \geq \theta(\mathbf{u}, \mathbf{v}).$$

Proof. Since $\mathbf{x} \in X$,

$$\begin{aligned} \theta(\mathbf{u}, \mathbf{v}) &= \inf_{\mathbf{y} \in X} \left(f(\mathbf{y}) + \mathbf{u}^T \mathbf{g}(\mathbf{y}) + \mathbf{v}^T \mathbf{h}(\mathbf{y}) \right) \\ &\leq f(\mathbf{x}) + \mathbf{u}^T \mathbf{g}(\mathbf{x}) + \mathbf{v}^T \mathbf{h}(\mathbf{x}) \\ &\leq f(\mathbf{x}), \end{aligned}$$

since $\mathbf{u} \geq \mathbf{0}, \mathbf{g}(\mathbf{x}) \leq \mathbf{0}$ and $\mathbf{h}(\mathbf{x}) = \mathbf{0}$. □

Corollaries of the Weak Duality Theorem

- $\inf\{f(\mathbf{x}) \mid \mathbf{x} \in X, \mathbf{g}(\mathbf{x}) \leq \mathbf{0}, \mathbf{h}(\mathbf{x}) = \mathbf{0}\} \geq \sup\{\theta(\mathbf{u}, \mathbf{v}) \mid \mathbf{u} \geq \mathbf{0}\}$.
- If $f(\bar{\mathbf{x}}) \leq \theta(\bar{\mathbf{u}}, \bar{\mathbf{v}})$, where $\bar{\mathbf{u}} \geq \mathbf{0}$ and $\bar{\mathbf{x}} \in \{\mathbf{x} \in X, \mathbf{g}(\mathbf{x}) \leq \mathbf{0}, \mathbf{h}(\mathbf{x}) = \mathbf{0}\}$, then $\bar{\mathbf{x}}$ and $(\bar{\mathbf{u}}, \bar{\mathbf{v}})$ solve the primal and dual problems respectively.
- If $\inf\{f(\mathbf{x}) \mid \mathbf{x} \in X, \mathbf{g}(\mathbf{x}) \leq \mathbf{0}, \mathbf{h}(\mathbf{x}) = \mathbf{0}\} = -\infty$, then $\theta(\mathbf{u}, \mathbf{v}) = -\infty$ for all $\mathbf{u} \geq \mathbf{0}, \mathbf{v} \in \mathbb{R}^k$.
- If $\sup\{\theta(\mathbf{u}, \mathbf{v}) \mid \mathbf{u} \geq \mathbf{0}\} = +\infty$, then the primal problem has no feasible solution.

Strong Duality Theorem

Assume that

- X : a nonempty convex set in $\mathbb{R}^n$;
- $f : X \to \mathbb{R}$ and $\mathbf{g} : X \to \mathbb{R}^m$: convex functions on X;
- $\mathbf{h} : \mathbb{R}^n \to \mathbb{R}^k$: an affine function, i.e., $\mathbf{h}(\mathbf{x}) = A\mathbf{x} - \mathbf{b}$ for some $k \times n$ matrix A and some vector $\mathbf{b}$ in $\mathbb{R}^k$;
  - Without loss of generality, we may assume that the matrix A has full rank.
- $\mathbf{0} \in \text{int } \mathbf{h}(X)$, where $\mathbf{h}(X) = \{\mathbf{h}(\mathbf{x}) : \mathbf{x} \in X\}$;
- there exists an $\mathbf{x}' \in X$ such that $\mathbf{g}(\mathbf{x}') < \mathbf{0}$ and $\mathbf{h}(\mathbf{x}') = \mathbf{0}$.

Then we have

$$\inf\{f(\mathbf{x}) : \mathbf{x} \in X, \mathbf{g}(\mathbf{x}) \leq \mathbf{0}, \mathbf{h}(\mathbf{x}) = \mathbf{0}\} = \sup\{\theta(\mathbf{u}, \mathbf{v}) : \mathbf{u} \geq \mathbf{0}\}.$$

Furthermore, if the inf is finite, then $\sup\{\theta(\mathbf{u},\mathbf{v}) \mid \mathbf{u} \geq \mathbf{0}\}$ is achieved at some $(\bar{\mathbf{u}},\bar{\mathbf{v}})$ with $\bar{\mathbf{u}} \geq \mathbf{0}$. If the inf is achieved at $\bar{\mathbf{x}}$, then $\sum_{i=1}^{m} \bar{u}_i g_i(\bar{\mathbf{x}}) = 0$.

Justification of Strong Duality for SVM

- $X = \mathbb{R}^N \times \mathbb{R}$: a non-empty convex set.
- $F(\mathbf{w}, b) = \frac{1}{2}\|\mathbf{w}\|^2$: a convex function on X.
- $g_i(\mathbf{w}, b) = 1 - c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b), 1 \leq i \leq m$: affine functions so that they are convex functions on X.
- There exists an $(\mathbf{w}', b') \in X$ such that $\mathbf{g}(\mathbf{w}', b') < \mathbf{0}$.

Then we have

$$\inf\{F(\mathbf{w}, b) : (\mathbf{w}, b) \in X, \mathbf{g}(\mathbf{w}, b) \leq \mathbf{0}\} = \sup\{\theta(\lambda) : \lambda \geq \mathbf{0}\}.$$

- For a linearly separable labeled training sample, the inf is finite and can be achieved at some feasible point $(\mathbf{w}^{SVM}, b^{SVM})$. Then $\sup\{\theta(\lambda) \mid \lambda \geq \mathbf{0}\}$ is achieved at some $\lambda^{SVM} \geq \mathbf{0}$.
- The primal and dual problems are equivalent.

The SVM Algorithm - Separable Case

- $S = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m)$: a linearly separable labeled training sample of size m with labels $(c(\mathbf{x}_1), c(\mathbf{x}_2), \ldots, c(\mathbf{x}_m))$.
- h_S^{SVM}: the hypothesis returned by SVM,

$$
\begin{aligned}
h_S^{SVM}(\mathbf{x}) &= \operatorname{sgn}(\mathbf{w}^{SVM} \cdot \mathbf{x} + b^{SVM}) \\
&= \operatorname{sgn}\Big(\sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)(\mathbf{x}_i \cdot \mathbf{x}) + b^{SVM}\Big)
\end{aligned}
$$

- $b^{SVM} = c(\mathbf{x}_j) - \sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)(\mathbf{x}_i \cdot \mathbf{x}_j)$ for any support vector $\mathbf{x}_j$. Thus we have

$$
h_S^{SVM}(\mathbf{x}) = \operatorname{sgn}\Big(c(\mathbf{x}_j) + \sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)(\mathbf{x}_i \cdot (\mathbf{x} - \mathbf{x}_j))\Big)
$$

for any support vector $\mathbf{x}_j$.

- The hypothesis solution h_S^{SVM} depends only on inner products between vectors and not directly on the vectors themselves.

The Maximum Margin $\rho_{\max}$

- $b^{SVM} = c(\mathbf{x}_j) - \sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)(\mathbf{x}_i \cdot \mathbf{x}_j)$ for any support vector $\mathbf{x}_j$. This implies

$$\begin{aligned} & \sum_{j=1}^{m} \lambda_j^{SVM} c(\mathbf{x}_j) b^{SVM} \\ = \; & \sum_{j=1}^{m} \lambda_j^{SVM} c(\mathbf{x}_j)^2 - \sum_{j=1}^{m} \lambda_j^{SVM} c(\mathbf{x}_j) \sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)(\mathbf{x}_i \cdot \mathbf{x}_j). \end{aligned}$$

- Since $\sum_{j=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_j) = 0$ and $\mathbf{w}^{SVM} = \sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)\mathbf{x}_i$, we have

$$\sum_{j=1}^{m} \lambda_j^{SVM} = \|\mathbf{w}^{SVM}\|^2.$$

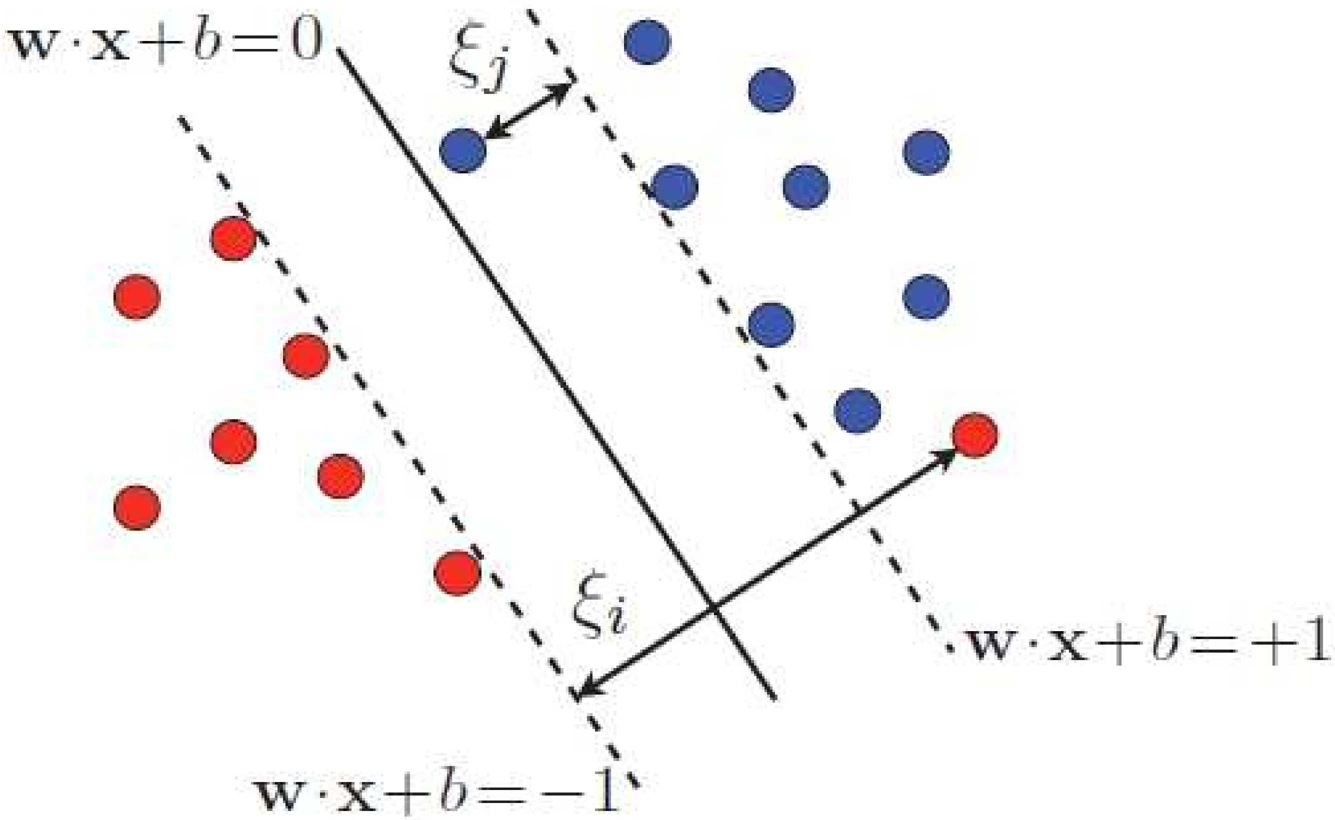
- $\rho_{\max}^2 = \frac{1}{\|\mathbf{w}^{SVM}\|^2} = \frac{1}{\sum_{j=1}^{m} \lambda_j^{SVM}}$.

The Contents of This Lecture

- Support vector machines - separable case.
- Support vector machines - general case.
- Margin guarantees.

Non-Linearly Separable Labeled Training Samples

- $S = (\mathbf{x}_1, \ldots, \mathbf{x}_m)$: a labeled training sample of m items, drawn i.i.d. from the input space according to P, with labels $(c(\mathbf{x}_1), \ldots, c(\mathbf{x}_m))$.
- Problem: the training data S is often not linearly separable in practice, i.e., for any hyperplane $\mathbf{w} \cdot \mathbf{x} + b = 0$, there exists $\mathbf{x}_i \in S$ such that
$$c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b) \not\geq 1.$$
- Idea: relax inequality constraints using slack variables $\eta_i \geq 0$, $i = 1, 2, \ldots, m$, such that
$$c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 - \eta_i.$$
  - A slack variable η_i measures the amount by which vector $\mathbf{x}_i$ violates the desired inequality $c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1$.



Point $\mathbf{x}_i$ is classified incorrectly and point $\mathbf{x}_j$ is correctly classified, but with a margin less than 1.

Remarks

- Soft margin : $\rho = 1/\|\mathbf{w}\|$.
- For a hyperplane $\mathbf{w} \cdot \mathbf{x} + b = 0$, a vector $\mathbf{x}_i$ with $\eta_i > 0$ can be viewed as an outlier.
- How should we select the hyperplane in the general, separable or non-separable, case?
- There are two conflicting objectives: on one hand, we wish to limit the total amount of slack due to outliers, which can be measured by $\sum_{i=1}^{m} \eta_i$ or $\sum_{i=1}^{m} \eta_i^p$ for some $p \geq 1$; on the other hand, we seek a hyperplane with a large soft margin, though a larger soft margin can lead to more outliers and thus larger amounts of slack.

The Primal Problem for SVM - General Case

$$
\begin{array}{ll}
\text{Minimize} & F(\mathbf{w}, b, \eta) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m} \eta_i \\
\text{Subject to} & 1 - \eta_i - c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b) \leq 0, i = 1, \ldots, m \\
 & -\eta_i \leq 0, i = 1, \ldots, m \\
 & (\mathbf{w}, b, \eta) \in \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^m.
\end{array}
$$

- A quadratic programming (QP) problem.

Remarks

- The parameter $C > 0$ determines the trade-off between margin-maximization (or minimization of $\|w\|^2$) and the minimization of the slack penalty $\sum_{i=1}^{m} \eta_i$.
- The parameter C is typically determined via n-fold cross-validation.

Qualification of the Primal Problem - General Case

- The object function $F(\mathbf{w}, b, \eta) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m}\eta_i$ is infinitely differentiable and convex so that it is pseudoconvex at any feasible point.

- The inequality constraint functions $g_i(\mathbf{w}, b, \eta) = 1 - \eta_i - c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b)$ and $h_i(\mathbf{w}, b, \eta) = -\eta_i$, $1 \leq i \leq m$, are affine functions so that they are infinitely differentiable and convex and then quasiconvex at any feasible point.

- $\nabla F = \begin{bmatrix} \mathbf{w} \\ 0 \\ C\mathbf{1} \end{bmatrix}$, $\nabla g_i = \begin{bmatrix} -c(\mathbf{x}_i)\mathbf{x}_i \\ -c(\mathbf{x}_i) \\ -\mathbf{e}_i \end{bmatrix}$, and $\nabla h_i = \begin{bmatrix} \mathbf{0} \\ 0 \\ -\mathbf{e}_i \end{bmatrix}$.

- The Kuhn-Tucker necessary conditions are:

$$\nabla F + \sum_{i=1}^{m} \lambda_i \nabla g_i + \sum_{i=1}^{m} \mu_i \nabla h_i = \mathbf{0}$$

$$\Leftrightarrow \mathbf{w} = \sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i)\mathbf{x}_i, 0 = \sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i), C = \lambda_i + \mu_i, i \in [1, m]$$

$$\lambda_i g_i(\mathbf{w}, b, \eta) = 0, \;\; i \in [1, m]$$

$$\mu_i \eta_i = 0, \;\; i \in [1, m]$$

$$\lambda_i, \mu_i \geq 0, \;\; i \in [1, m].$$

- Any feasible point $(\mathbf{w}, b, \eta)$ which satisfies the Kuhn-Tucker necessary conditions in above is a global minimum solution.
- The weight vector $\mathbf{w}$ solution of the general, separable or non-separable, SVM problem is also a linear combination of the training set vectors $\mathbf{x}_1, \ldots, \mathbf{x}_m$.

Support Vectors

- Support vectors: any vector $\mathbf{x}_i$ which appears in the linear combination $\mathbf{w} = \sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i)\mathbf{x}_i$, i.e., $\lambda_i \neq 0$.
- If $\lambda_i \neq 0$, we must have $c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b) = 1 - \eta_i$ by the complementary slackness conditions.
- If $\eta_i = 0$, the support vector $\mathbf{x}_i$ lies in the marginal hyperplane $\mathbf{w} \cdot \mathbf{x} + b = c(\mathbf{x}_i)$.
- If $\eta_i > 0$, the support vector $\mathbf{x}_i$ is an outlier. In this case, $\mu_i = 0$ and then $\lambda_i = C$.

Remarks

- Support vectors fully define the maximum-margin hyperplane or SVM solution.
- Support vectors $\mathbf{x}_i$ are either outliers, in which case λ_i must be C, or vectors lying on the marginal hyperplanes.
- Vectors in the sample neither outliers nor lying on the marginal hyperplanes do not affect the solution to the SVM problem.
- As in the separable case, note that while the solution $\mathbf{w}$ of the SVM problem is usually unique, the support vectors are not.

How to Determine Optimal Lagrangian Variables λ_i^{SVM} ?

- Once optimal Lagrangian variables λ_i^{SVM} are determined, we can compute

$$\mathbf{w}^{SVM} = \sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)\mathbf{x}_i$$

  and for any support vector $\mathbf{x}_j$ lying on the marginal hyperplanes, we have

$$b^{SVM} = c(\mathbf{x}_j) - \mathbf{w}^{SVM} \cdot \mathbf{x}_j = c(\mathbf{x}_j) - \sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)(\mathbf{x}_i \cdot \mathbf{x}_j).$$

- We will use the Lagrangian dual problem to determine optimal λ_i^{SVM}.

Lagrangian Dual Function for SVM - General Case

- $X = \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^m$: a nonempty open convex set.
- Lagrangian function: for all $\mathbf{w} \in \mathbb{R}^N, b \in \mathbb{R}, \eta \in \mathbb{R}^m$, and $\lambda \in \mathbb{R}^m, \mu \in \mathbb{R}^m$,

$$
\begin{aligned}
& L(\mathbf{w}, b, \eta, \lambda, \mu) \\
= \quad & F(\mathbf{w}, b, \eta) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{w}, b, \eta) + \sum_{i=1}^{m} \mu_i h_i(\mathbf{w}, b, \eta) \\
= \quad & \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m} \eta_i + \sum_{i=1}^{m} \lambda_i (1 - \eta_i - c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b)) \\
& - \sum_{i=1}^{m} \mu_i \eta_i.
\end{aligned}
$$

- For any fixed $\lambda, \mu \in \mathbb{R}^m$, the gradient ∇L of the Lagrangian function w.r.t. $(\mathbf{w}, b, \eta)$ is

$$
\begin{aligned}
\nabla L &= \nabla F + \sum_{i=1}^{m} \lambda_i \nabla g_i + \sum_{i=1}^{m} \mu_i \nabla h_i \\
&= \begin{bmatrix} \mathbf{w} \\ 0 \\ C\mathbf{1} \end{bmatrix} - \sum_{i=1}^{m} \lambda_i \begin{bmatrix} c(\mathbf{x}_i)\mathbf{x}_i \\ c(\mathbf{x}_i) \\ \mathbf{e}_i \end{bmatrix} - \sum_{i=1}^{m} \mu_i \begin{bmatrix} \mathbf{0} \\ 0 \\ \mathbf{e}_i \end{bmatrix}
\end{aligned}
$$

and the Hessian matrix is

$$
\mathbf{H} = \begin{bmatrix} I_{N\times N} & \mathbf{0}_{N\times(m+1)} \\ \mathbf{0}_{(m+1)\times N} & \mathbf{0}_{(m+1)\times(m+1)} \end{bmatrix}
$$

which is positive semi-definite.

- For any fixed $\lambda, \mu \in \mathbb{R}^m$, the Lagrangian function is differentiable and convex over a non-empty open convex set X so that $(\hat{\mathbf{w}}, \hat{b}, \hat{\eta})$ is an optimal solution to the minimization of $L(\mathbf{w}, b, \eta, \lambda, \mu)$ subject to $(\mathbf{w}, b, \eta) \in X$ if and only if $\nabla L(\hat{\mathbf{w}}, \hat{b}, \hat{\eta}, \lambda, \mu) = \mathbf{0}$ if and only if

$$\hat{\mathbf{w}} = \sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i)\mathbf{x}_i,\ 0 = \sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i),\ \text{ and }\ C = \lambda_i + \mu_i,\ i \in [1, m].$$

  - Note that for any fixed $\lambda, \mu \in \mathbb{R}^m$, $\sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i) \neq 0$ or $C \neq \lambda_i + \mu_i$ for some $i \in [1, m]$ if and only if the infimum of the Lagrangian function $L(\mathbf{w}, b, \eta, \lambda, \mu)$ is $-\infty$.

- Lagrangian dual function: for any $\lambda, \mu \in \mathbb{R}^m$,

$$
\begin{aligned}
& \theta(\lambda, \mu) \\
= \quad & \inf_{(\mathbf{w}, b, \eta) \in X} L(\mathbf{w}, b, \eta, \lambda, \mu) \\
= \quad & \begin{cases} \frac{1}{2}\|\hat{\mathbf{w}}\|^2 + C \sum_{i=1}^m \hat{\eta}_i + \sum_{i=1}^m \lambda_i (1 - \hat{\eta}_i - c(\mathbf{x}_i)(\hat{\mathbf{w}} \cdot \mathbf{x}_i + \hat{b})) \\ - \sum_{i=1}^m \mu_i \hat{\eta}_i, \text{ if } \sum_{i=1}^m \lambda_i c(\mathbf{x}_i) = 0, C = \lambda_i + \mu_i, i \in [1, m], \\ -\infty, \text{ otherwise} \end{cases} \\
= \quad & \begin{cases} \sum_{i=1}^m \lambda_i - \frac{1}{2} \sum_{i,j=1}^m \lambda_i \lambda_j c(\mathbf{x}_i) c(\mathbf{x}_j)(\mathbf{x}_i \cdot \mathbf{x}_j), \\ \qquad\qquad \text{if } \sum_{i=1}^m \lambda_i c(\mathbf{x}_i) = 0, , C = \lambda_i + \mu_i, i \in [1, m], \\ -\infty, \text{ otherwise.} \end{cases}
\end{aligned}
$$

Lagrangian Dual Problem for SVM - General Case

Maximize $\theta(\lambda, \mu) = \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j c(\mathbf{x}_i) c(\mathbf{x}_j)(\mathbf{x}_i \cdot \mathbf{x}_j)$

Subject to $\lambda_i, \mu_i \geq 0, i = 1, \ldots, m$

$\lambda_i + \mu_i - C = 0, i = 1, \ldots, m$

$\sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i) = 0$

$(\lambda, \mu) \in \mathbb{R}^m \times \mathbb{R}^m$

Or equivalently,

$$
\begin{array}{ll}
\text{Maximize} & \theta(\lambda) = \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j c(\mathbf{x}_i) c(\mathbf{x}_j)(\mathbf{x}_i \cdot \mathbf{x}_j) \\
\text{Subject to} & \lambda_i \geq 0, i = 1, \ldots, m \\
 & C - \lambda_i \geq 0, i = 1, \ldots, m \\
 & \sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i) = 0 \\
 & \lambda \in \mathbb{R}^m
\end{array}
$$

- A quadratic programming (QP) problem.

Qualification of the Dual Problem

- The object function

$$\theta(\lambda) = \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j c(\mathbf{x}_i) c(\mathbf{x}_j)(\mathbf{x}_i \cdot \mathbf{x}_j)$$

  is infinitely differentiable and concave so that it is pseudoconcave at any feasible point.

- The inequality constraint functions $g_i(\lambda) = \lambda_i, 1 \leq i \leq m$, $\tilde{g}_i(\lambda) = C - \lambda_i, 1 \leq i \leq m$, and the equality constraint function $h(\lambda) = \sum_{i=1}^{m} \lambda_i c(\mathbf{x}_i)$ are affine functions so that they are infinitely differentiable, concave and convex and then quasiconcave and quasiconvex at any feasible point.

- $\nabla\theta(\lambda) = \mathbf{1} - \mathbf{A}\lambda$, where $\mathbf{A} = [c(\mathbf{x}_i)\mathbf{x}_i \cdot c(\mathbf{x}_j)\mathbf{x}_j]$ is the Gram matrix of the vectors $c(\mathbf{x}_i)\mathbf{x}_i, 1 = 1, 2, \ldots, m$.
- $\nabla g_i(\lambda) = \mathbf{e}_i, i = 1, 2, \ldots, m$, $\nabla \tilde{g}_i(\lambda) = -\mathbf{e}_i, i = 1, 2, \ldots, m$, and $\nabla h(\lambda) = [c(\mathbf{x}_1), \ldots, c(\mathbf{x}_m)]^T$.
- The Kuhn-Tucker necessary conditions are:

$$\nabla\theta + \sum_{i=1}^{m} u_i \nabla g_i + \sum_{i=1}^{m} \tilde{u}_i \nabla \tilde{g}_i + v\nabla h = \mathbf{0}$$

$$\Leftrightarrow \mathbf{A}\lambda = \mathbf{1} + \mathbf{u} - \tilde{\mathbf{u}} + v \begin{bmatrix} c(\mathbf{x}_1) \\ \vdots \\ c(\mathbf{x}_m) \end{bmatrix}$$

$$u_i\lambda_i = 0, \tilde{u}_i(C - \lambda_i) = 0, \ i = 1, 2, \ldots, m$$

$$u_i, \tilde{u}_i \geq 0, \ i = 1, 2, \ldots, m.$$

- Any feasible point λ which satisfies the Kuhn-Tucker necessary conditions in above is a global maximum solution.

Justification of Strong Duality for SVM - General Case

- $X = \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^m$: a non-empty convex set.
- $F(\mathbf{w}, b, \eta) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^m \eta_i$: a convex function on X.
- $g_i(\mathbf{w}, b, \eta) = 1 - \eta_i - c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i + b), 1 \leq i \leq m$: affine functions so that they are convex functions on X.
- $h_i(\mathbf{w}, b, \eta) = -\eta_i, 1 \leq i \leq m$: affine functions so that they are convex functions on X.
- There exists an $(\mathbf{w}', b', \eta') \in X$ such that $\mathbf{g}(\mathbf{w}', b', \eta') < \mathbf{0}$ and $\mathbf{h}(\mathbf{w}', b', \eta') < \mathbf{0}$.

Then we have

$$\begin{aligned} & \inf\{F(\mathbf{w}, b, \eta) : (\mathbf{w}, b, \eta) \in X, \mathbf{g}(\mathbf{w}, b, \eta) \leq \mathbf{0}, \mathbf{h}(\mathbf{w}, b, \eta) \leq \mathbf{0}\} \\ = \quad & \sup\{\theta(\lambda, \mu) : (\lambda, \mu) \geq \mathbf{0}\}. \end{aligned}$$

- For a non-trivial labeled training sample, the inf is finite and can be achieved at some feasible point $(\mathbf{w}^{SVM}, b^{SVM}, \eta^{SVM})$. Then $\sup\{\theta(\lambda) \mid \lambda \geq \mathbf{0}\}$ is achieved at some $(\lambda^{SVM}, \mu^{SVM}) \geq \mathbf{0}$.
- The primal and dual problems are equivalent.

The SVM Algorithm - General Case

- $S = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m)$: a non-trivial labeled training sample of size m with labels $(c(\mathbf{x}_1), c(\mathbf{x}_2), \ldots, c(\mathbf{x}_m))$.
- h_S^{SVM}: the hypothesis returned by SVM,

$$\begin{aligned} h_S^{SVM}(\mathbf{x}) &= \mathrm{sgn}(\mathbf{w}^{SVM} \cdot \mathbf{x} + b^{SVM}) \\ &= \mathrm{sgn}(\sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)(\mathbf{x}_i \cdot \mathbf{x}) + b^{SVM}) \end{aligned}$$

- $b^{SVM} = c(\mathbf{x}_j) - \sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)(\mathbf{x}_i \cdot \mathbf{x}_j)$ for any support vector $\mathbf{x}_j$ with $0 < \lambda_j < C$. Thus we have

$$h_S^{SVM}(\mathbf{x}) = \mathrm{sgn}(c(\mathbf{x}_j) + \sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)(\mathbf{x}_i \cdot (\mathbf{x} - \mathbf{x}_j)))$$

for any support vector $\mathbf{x}_j$ with $0 < \lambda_j < C$.

- The hypothesis solution h_S^{SVM} depends only on inner products between vectors and not directly on the vectors themselves.

The SVM Soft Margin ρ_{SVM}

- $b^{SVM} = c(\mathbf{x}_j) - c(\mathbf{x}_j)\eta_j^{SVM} - \sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)(\mathbf{x}_i \cdot \mathbf{x}_j)$ for any support vector $\mathbf{x}_j$, i.e., $\lambda_j^{SVM} > 0$. This implies

$$
\begin{aligned}
& \sum_{j=1}^{m} \lambda_j^{SVM} c(\mathbf{x}_j) b^{SVM} \\
= \quad & \sum_{j=1}^{m} \lambda_j^{SVM} (1 - \eta_j^{SVM}) c(\mathbf{x}_j)^2 \\
& - \sum_{j=1}^{m} \lambda_j^{SVM} c(\mathbf{x}_j) \sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)(\mathbf{x}_i \cdot \mathbf{x}_j).
\end{aligned}
$$

- Since $\sum_{j=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_j) = 0$ and $\mathbf{w}^{SVM} = \sum_{i=1}^{m} \lambda_i^{SVM} c(\mathbf{x}_i)\mathbf{x}_i$, we have

$$\sum_{j=1}^{m} \lambda_j^{SVM}(1 - \eta_j^{SVM}) = \|\mathbf{w}^{SVM}\|^2.$$

- ${\rho_{SVM}}^2 = \frac{1}{\|\mathbf{w}^{SVM}\|^2} = \frac{1}{\sum_{j=1}^{m} \lambda_j^{SVM}(1-\eta_j^{SVM})}.$

The Contents of This Lecture

- Support vector machines - separable case.
- Support vector machines - non-separable case.
- Margin guarantees.

Binary Linear Classification Problem

- $\mathscr{I} \subseteq \mathbb{R}^N$: the input space.
- $\mathscr{Y}' = \mathscr{Y} = \{-1, +1\}$: the output, label space with loss function $L(y', y) = 1_{y' \neq y}$.
- c: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- $\mathcal{H} = \{\mathbf{x} \mapsto \operatorname{sgn}(\mathbf{w} \cdot \mathbf{x} + b) \mid \mathbf{w} \in \mathbb{R}^N,\ b \in \mathbb{R}\}$: the hypothesis set of all linear classifiers.
- $S = (\mathbf{x}_1, \ldots, \mathbf{x}_m)$: a sample of m items, drawn i.i.d. from the input space according to P, with labels $(c(\mathbf{x}_1), \ldots, c(\mathbf{x}_m))$.
- Problem: find a linear hypothesis (binary linear classifier) $h : \mathscr{I} \to \{-1, +1\}$ in $\mathcal{H}$ with small generalization error

$$R(h) = E[1_{h(\mathbf{x}) \neq c(\mathbf{x})}] = P(h(\mathbf{x}) \neq c(\mathbf{x})).$$

VC-Dimension Generalization Bound - Binary Linear Classification

- $\mathscr{I} \subseteq \mathbb{R}^N$: the input space, not contained in any hyperplane.
- $c : \mathscr{I} \to \{-1, +1\}$: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- $\mathcal{H} = \{\mathbf{x} \mapsto \operatorname{sgn}(\mathbf{w} \cdot \mathbf{x} + b) \mid \mathbf{w} \in \mathbb{R}^N,\ b \in \mathbb{R}\}$: the hypothesis set of all linear classifiers.
  - Since the input space $\mathscr{I}$ is not contained in any hyperplane, we cannot use linear classifiers in $\mathbb{R}^{N-1}$.
  - $\mathrm{VCdim}(\mathcal{H}) = N + 1$.
- $S = (\mathbf{x}_1, \ldots, \mathbf{x}_m)$: a sample of size m drawn i.i.d. from the input space $\mathscr{I}$ according to an unknown distribution P, with labels $(c(\mathbf{x}_1), \ldots, c(\mathbf{x}_m))$.

For any $\delta > 0$, with probability at least $1 - \delta$, we have

$$\forall\, h \in \mathcal{H}, \quad R(h) \leq \hat{R}_S(h) + \sqrt{\frac{2(N+1)\ln\frac{em}{N+1}}{m}} + \sqrt{\frac{\ln\frac{1}{\delta}}{2m}}.$$

Proof. This is a direct consequence of Corollary 3.4. $\square$

Remarks

- When the dimension N of the input space is large compared to the sample size m, this VC-dimension generalization bound is uninformative.
- Informative bound which does not depend on the dimension N of the input space will be derived.

Geometric Margin of a Point to a Linear Classifier

The geometric margin $\rho_h(\mathbf{x})$ of a point $\mathbf{x}$ in $\mathbb{R}^N$ with respect to a linear classifier $h : x \mapsto \mathrm{sgn}(\mathbf{w} \cdot \mathbf{x} + b)$ is its distance to the hyperplane $\mathbf{w} \cdot \mathbf{x} + b = 0$:

$$\rho_h(\mathbf{x}) = \frac{|\mathbf{w} \cdot \mathbf{x} + b|}{\|\mathbf{w}\|}.$$

Geometric Margin of a Finite Set of Points to a Linear Classifier

The geometric margin $\rho_h(A)$ of a finite set $A = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m\}$ of points in $\mathbb{R}^N$ with respect to a linear classifier $h : \mathbf{x} \mapsto \operatorname{sgn}(\mathbf{w} \cdot \mathbf{x} + b)$ is the minimum geometric margin over the points in the set:

$$\rho_h(A) = \min_{1 \le i \le m} \frac{|\mathbf{w} \cdot \mathbf{x_i} + b|}{\|\mathbf{w}\|}.$$

Canonical Representation of a Separating Linear Classifier to a Finite Set of Points

- $A = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m\}$: a finite set of points in $\mathbb{R}^N$.
- h: a separating linear classifier to A, i.e, no points of A being in the boundary hyperplane of h.

A representation $h : x \mapsto \mathrm{sgn}(\mathbf{w} \cdot \mathbf{x} + b)$ of the separating linear classifier h to the set A is called canonical to A if

$$\min_{1 \leq i \leq m} |\mathbf{w} \cdot \mathbf{x}_i + b| = 1.$$

The geometric margin of the set A with respective to the canonically represented separating linear classifier $h : \mathbf{x} \mapsto \mathrm{sgn}(\mathbf{w} \cdot \mathbf{x} + b)$ to A is

$$\rho_h(A) = \min_{1 \leq i \leq m} \frac{|\mathbf{w} \cdot \mathbf{x}_i + b|}{\|\mathbf{w}\|} = \frac{1}{\|\mathbf{w}\|}.$$

VC-Dimension of a Family of Separating Linear Classifiers to a Finite Input Space with Margin Guarantee

Theorem 4.2: Let

- $A \subseteq \mathbb{R}^N$: a finite input space with $r \triangleq \max_{\mathbf{x}\in A} \|\mathbf{x}\|_2$.
- $\mathcal{H}$: the family of all separating linear classifiers to A with geometric margin at least $1/\Lambda$ whose boundary hyperplane contains the origin $\mathbf{0}$, i.e.,

$$\mathcal{H} = \{\mathbf{x} \mapsto \mathrm{sgn}(\mathbf{w}\cdot\mathbf{x}) \mid \min_{\mathbf{x}\in A} |\mathbf{w}\cdot\mathbf{x}_i| = 1 \text{ and } \|\mathbf{w}\| \le \Lambda\}.$$

  - Every separating hyperplane to the input space A has a unique canonical representation to A up to ± 1.
  - Each linear classifier (hypothesis) h in $\mathcal{H}$ is a function from the input space A to the output (label) space $\{-1, +1\}$.

Then $d = \mathrm{VC}\ \dim(\mathcal{H}) \le r^2\Lambda^2$.

Proof. Assume

- $B = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_d\}$: a d-subset of A that can be shattered by $\mathcal{H}$;
- $\mathbf{y} = (y_1, y_2, \ldots, y_d) \in \{-1, +1\}^d$: a dichotomy of B;
- $\mathbf{x} \mapsto \operatorname{sgn}(\mathbf{w}_\mathbf{y} \cdot \mathbf{x})$: a linear classifier in $\mathcal{H}$ which realizes the dichotomy $\mathbf{y}$ of B.
  - $\mathbf{w}_\mathbf{y}$ depends on $\mathbf{y}$.

Then we have

$$1 \le y_i(\mathbf{w}_\mathbf{y} \cdot \mathbf{x}_i) \ \forall\ i \in [1, d]$$

and, summing up over i, yield

$$d \le \mathbf{w}_\mathbf{y} \cdot \sum_{i=1}^{d} y_i \mathbf{x}_i \le \|\mathbf{w}_\mathbf{y}\| \left\| \sum_{i=1}^{d} y_i \mathbf{x}_i \right\| .$$

By taking equally weighted sum over all possible dichotomies $\mathbf{y}$ and noting that $\|\mathbf{w}_{\mathbf{y}}\| \leq \Lambda$, we have

$$
\begin{aligned}
d &\leq \Lambda \sum_{\mathbf{y}\in\{-1,+1\}^d} \frac{1}{2^d} \sqrt{\sum_{i=1}^{d} y_i \mathbf{x}_i \cdot \sum_{j=1}^{d} y_j \mathbf{x}_j} \\
&\leq \Lambda \sqrt{\sum_{\mathbf{y}\in\{-1,+1\}^d} \frac{1}{2^d} \sum_{i,j=1}^{d} y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j)} \\
&\qquad \text{since } f(x) = \sqrt{x} \text{ is a concave function on } [0,\infty) \\
&= \Lambda \sqrt{\sum_{i,j=1}^{d} (\mathbf{x}_i \cdot \mathbf{x}_j) \frac{1}{2^d} \sum_{\mathbf{y}\in\{-1,+1\}^d} y_i y_j} \\
&= \Lambda \sqrt{\sum_{i=1}^{d} (\mathbf{x}_i \cdot \mathbf{x}_i)} \\
&\leq \Lambda \sqrt{d r^2} = \Lambda r \sqrt{d}
\end{aligned}
$$

since

$$\frac{1}{2^d} \sum_{\mathbf{y} \in \{-1,+1\}^d} y_i y_j = \begin{cases} 0, & \text{if } i \neq j, \\ 1, & \text{if } i = j. \end{cases}$$

Thus we have $d \leq \Lambda^2 r^2$. $\square$

Rademacher Complexity of a Family of Linear Functions on Bounded Input Space with Bounded Weight Vector

Theorem 4.3: Let

- $\mathscr{I} = \bar{B}(r;\mathbf{0}) = \{\mathbf{x} : \|\mathbf{x}\| \leq r\} \subseteq \mathbb{R}^N$: the bounded input space, associated with a probability space $(\bar{B}(r;\mathbf{0}), \mathcal{F}, P)$.
- $\mathcal{H} = \{\mathbf{x} \mapsto \mathbf{w} \cdot \mathbf{x} \mid \|\mathbf{w}\| \leq \Lambda\}$: the family of all linear functions with bounded weight vector.
- $S = (\mathbf{x}_1, \ldots, \mathbf{x}_m)$: a sample of m points drawn i.i.d. from the input space $\bar{B}(r;\mathbf{0})$ according to an unknown distribution P.

Then the empirical Rademacher complexity of $\mathcal{H}$ w.r.t. the sample S can be upper bounded as follows:

$$\hat{\mathfrak{R}}_S(\mathcal{H}) \leq \sqrt{\frac{r^2\Lambda^2}{m}}.$$

Proof.

$$
\begin{aligned}
\hat{\mathfrak{R}}_S(\mathcal{H}) &= \frac{1}{2^m} \sum_{\sigma_1,\sigma_2,\ldots,\sigma_m \in \{-1,+1\}} \sup_{h \in \mathcal{H}} \frac{1}{m} \sum_{i=1}^{m} \sigma_i h(\mathbf{x}_i) \\
&= \frac{1}{2^m} \sum_{\sigma_1,\sigma_2,\ldots,\sigma_m \in \{-1,+1\}} \sup_{\|\mathbf{w}\| \leq \Lambda} \frac{1}{m} \sum_{i=1}^{m} \sigma_i (\mathbf{w} \cdot \mathbf{x}_i) \\
&= \frac{1}{2^m} \sum_{\sigma_1,\sigma_2,\ldots,\sigma_m \in \{-1,+1\}} \sup_{\|\mathbf{w}\| \leq \Lambda} \frac{1}{m} \mathbf{w} \cdot \sum_{i=1}^{m} \sigma_i \mathbf{x}_i \\
&\leq \frac{\Lambda}{m} \sum_{\sigma_1,\sigma_2,\ldots,\sigma_m \in \{-1,+1\}} \frac{1}{2^m} \sqrt{\sum_{i=1}^{d} \sigma_i \mathbf{x}_i \cdot \sum_{j=1}^{d} \sigma_j \mathbf{x}_j} \\
&\leq \frac{\Lambda}{m} \sqrt{\sum_{\sigma_1,\sigma_2,\ldots,\sigma_m \in \{-1,+1\}} \frac{1}{2^m} \sum_{i,j=1}^{m} \sigma_i \sigma_j (\mathbf{x}_i \cdot \mathbf{x}_j)},
\end{aligned}
$$

again since $f(x) = \sqrt{x}$ is a concave function on $[0, \infty)$. Now we have

$$
\begin{aligned}
\hat{\mathfrak{R}}_S(\mathcal{H}) &\leq \frac{\Lambda}{m}\sqrt{\sum_{i,j=1}^{m}(\mathbf{x}_i\cdot\mathbf{x}_j)\frac{1}{2^m}\sum_{\sigma_1,\sigma_2,\ldots,\sigma_m\in\{-1,+1\}}\sigma_i\sigma_j} \\
&= \frac{\Lambda}{m}\sqrt{\sum_{i=1}^{m}(\mathbf{x}_i\cdot\mathbf{x}_i)} \\
&\leq \frac{\Lambda}{m}\sqrt{mr^2} = \sqrt{\frac{\Lambda^2 r^2}{m}}
\end{aligned}
$$

since

$$
\frac{1}{2^m}\sum_{\sigma_1,\sigma_2,\ldots,\sigma_m\in\{-1,+1\}}\sigma_i\sigma_j = \begin{cases} 0, & \text{if } i\neq j, \\ 1, & \text{if } i=j. \end{cases}
$$

Thus we have $\hat{\mathfrak{R}}_S(\mathcal{H}) \leq \sqrt{\frac{r^2\Lambda^2}{m}}$. $\square$

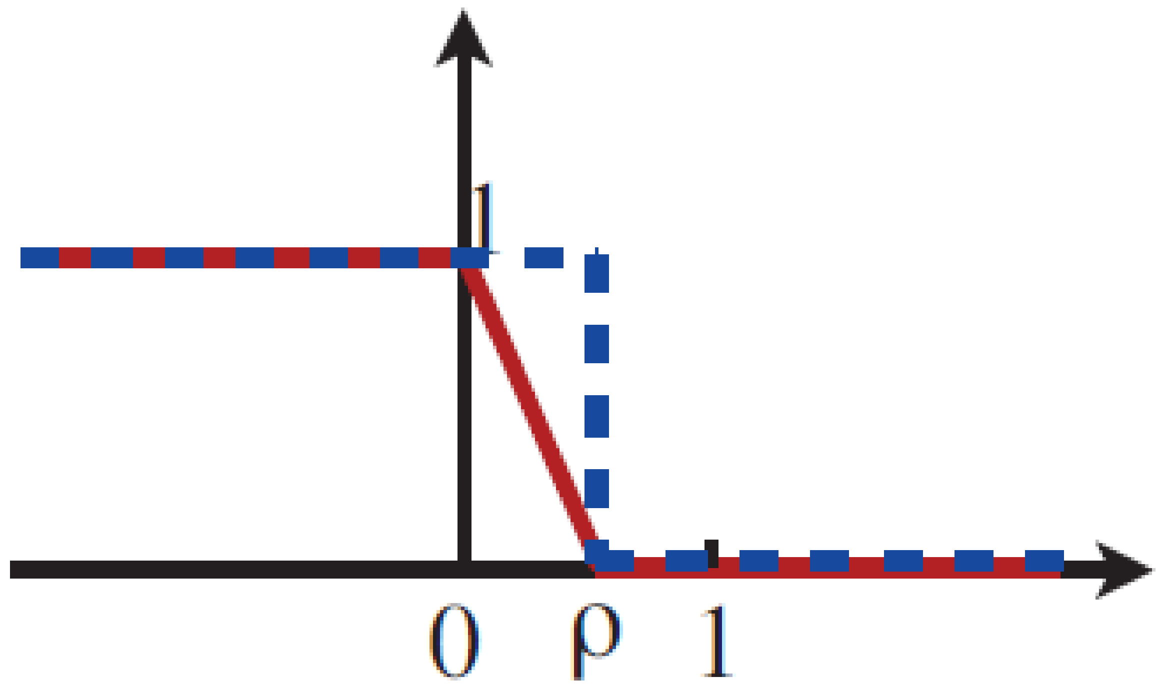
ρ-Margin Loss Function

- $\rho > 0$: a given confidence margin.
- $\Phi_\rho(x) : \mathbb{R} \to [0, 1]$: a soft inverse limiter with margin ρ, defined as

$$\Phi_\rho(x) = \begin{cases} 1, & \text{if } x \leq 0, \\ 1 - x/\rho, & \text{if } 0 \leq x \leq \rho, \\ 0, & \text{if } x \geq \rho. \end{cases}$$

The ρ-margin loss function $L_\rho : \mathbb{R} \times \mathbb{R} \to [0, 1]$ is defined as

$$L_\rho(y', y) \triangleq \Phi_\rho(y'y).$$



Three functions $\Phi_0(x) \leq \Phi_\rho(x)$(in red) $\leq \Phi_0(x-\rho)$(in blue) for constructing different loss functions.

Remarks

- When using a real-valued function h as a hypothesis to approximate a concept c which is a $\{-1, +1\}$-valued function, the 0-1 loss function used will be

$$L(y', y) = 1_{\mathrm{sgn}(y') \neq \mathrm{sgn}(y)} = 1_{y'y \leq 0} = \Phi_0(y'y),$$

where $\Phi_0(x)$ is the hard inverse limiter,

$$\Phi_0(x) = \begin{cases} 1, & \text{if } x \leq 0, \\ 0, & \text{if } x > 0. \end{cases}$$

- The 0-1 loss function $L(y', y) = 1_{y'y \leq 0}$ is always no greater than the ρ-margin loss function $L_\rho(y', y)$.

Empirical ρ-Margin Loss

- $\mathscr{I}$: the input space of all possible items ω, associated with a probability space $(\mathscr{I}, \mathcal{F}, P)$.
- $c : \mathscr{I} \to \{-1, +1\}$: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- $\mathscr{Y}'$: the output space, which is usually a bounded subset of $\mathbb{R}$.
- $\mathcal{H}$: a hypothesis set of $\mathscr{Y}'$-valued functions on the input space $\mathscr{I}$.
- $L_\rho(y', y) = \Phi_\rho(y'y)$: the ρ-margin loss function.
- $S = (\omega_1, \ldots, \omega_m)$: a sample of size m drawn i.i.d. from $\mathscr{I}$ according to an unknown distribution P, with labels $(c(\omega_1), \ldots, c(\omega_m))$.
- h: an arbitrary hypothesis in $\mathcal{H}$.

The empirical ρ-margin loss of an hypothesis h w.r.t. the concept c on the labeled sample S is defined as

$$\hat{R}_{S,\rho}(h) \triangleq \frac{1}{m}\sum_{i=1}^{m} L_\rho(h(\omega_i), c(\omega_i)) = \frac{1}{m}\sum_{i=1}^{m} \Phi_\rho(h(\omega_i)c(\omega_i)).$$

Remarks

- Since the 0-1 loss function $L(y', y) = 1_{y'y \le 0}$ is always no greater than the ρ-margin loss function $L_\rho(y', y)$, the empirical error is

$$\begin{aligned} \hat{R}_S(h) &= \frac{1}{m} \sum_{i=1}^{m} L(h(\omega_i), c(\omega_i)) \\ &\le \frac{1}{m} \sum_{i=1}^{m} L_\rho(h(\omega_i), c(\omega_i)) = \hat{R}_{S,\rho}(h). \end{aligned}$$

Talagrand's Lemma

Lemma 4.2: Let

- $\mathscr{I}$: the input space of all possible items ω, associated with a probability space $(\mathscr{I}, \mathcal{F}, P)$.
- $\mathscr{Y}' \subseteq \mathbb{R}$: the output space, which is a subset of $\mathbb{R}$.
- $\mathcal{H}$: a hypothesis set of $\mathscr{Y}'$-valued measurable functions on the input space $\mathscr{I}$.
- $\Phi : \mathscr{Y}' \to \mathbb{R}$: an α-Lipschitz function, i.e., there is an $\alpha > 0$ such that $|\Phi(x) - \Phi(y)| \leq \alpha |x - y|$, $\forall\ x, y \in \mathscr{Y}'$.
- $S = (\omega_1, \omega_2, \ldots, \omega_m)$: a sample of m items drawn i.i.d. from $\mathscr{I}$ according to P.

Assume that

- $\sup_{h\in\mathcal{H}} \left(\sum_{i=1}^{j} \sigma_i(\Phi \circ h)(\omega_i) + \sum_{i=j+1}^{m} \alpha\sigma_i h(\omega_i)\right)$ is finite for all $\sigma_i \in \{-1, +1\}, i \in [1, m]$ and for all $j \in [0, m]$.

Then we have

$$\hat{\mathfrak{R}}_S(\Phi \circ \mathcal{H}) \leq \alpha\hat{\mathfrak{R}}_S(\mathcal{H}),$$

where both $\hat{\mathfrak{R}}_S(\Phi \circ \mathcal{H})$ and $\hat{\mathfrak{R}}_S(\mathcal{H})$ are finite.

Proof. By the definition of empirical Rademacher complexity,

$$
\begin{aligned}
\hat{\mathfrak{R}}_S(\Phi \circ \mathcal{H}) &= \frac{1}{2^m} \sum_{\sigma_1, \sigma_2, \ldots, \sigma_m \in \{-1,+1\}} \sup_{h \in \mathcal{H}} \frac{1}{m} \sum_{i=1}^{m} \sigma_i (\Phi \circ h)(\omega_i) \\
&= \frac{1}{2^{m-1}} \sum_{\sigma_1, \sigma_2, \ldots, \sigma_{m-1} \in \{-1,+1\}} \frac{1}{2} \sum_{\sigma_m \in \{-1,+1\}} \frac{1}{m} \\
&\quad \sup_{h \in \mathcal{H}} \left(u_{m-1}(h) + \sigma_m (\Phi \circ h)(\omega_m) \right),
\end{aligned}
$$

where $u_{m-1}(h) \triangleq \sum_{i=1}^{m-1} \sigma_i (\Phi \circ h)(\omega_i)$. Since $\sup_{h \in \mathcal{H}} \sum_{i=1}^{m} \sigma_i (\Phi \circ h)(\omega_i)$ is finite for any given $\sigma_1, \sigma_2, \ldots, \sigma_m$ by assumption, for any $\epsilon > 0$, there exist $h_1, h_2 \in \mathcal{H}$ such that

$$
\begin{aligned}
\sup_{h \in \mathcal{H}} \left(u_{m-1}(h) + (\Phi \circ h)(\omega_m) \right) - \epsilon &\leq u_{m-1}(h_1) + (\Phi \circ h_1)(\omega_m), \\
\sup_{h \in \mathcal{H}} \left(u_{m-1}(h) - (\Phi \circ h)(\omega_m) \right) - \epsilon &\leq u_{m-1}(h_2) - (\Phi \circ h_2)(\omega_m)
\end{aligned}
$$

and then

$$
\begin{aligned}
& \frac{1}{2} \sum_{\sigma_m \in \{-1,+1\}} \sup_{h \in \mathcal{H}} \left(u_{m-1}(h) + \sigma_m (\Phi \circ h)(\omega_m) \right) - \epsilon \\
\leq \quad & \frac{1}{2} \left(u_{m-1}(h_1) + (\Phi \circ h_1)(\omega_m) \right) + \frac{1}{2} \left(u_{m-1}(h_2) - (\Phi \circ h_2)(\omega_m) \right) \\
\leq \quad & \frac{1}{2} \left(u_{m-1}(h_1) + u_{m-1}(h_2) + s\alpha(h_1(\omega_m) - h_2(\omega_m)) \right) \\
& \text{by Lipschitz property, where } s = \operatorname{sgn}(h_1(\omega_m) - h_2(\omega_m)) \\
= \quad & \frac{1}{2} \left(u_{m-1}(h_1) + s\alpha h_1(\omega_m) \right) + \frac{1}{2} \left(u_{m-1}(h_2) - s\alpha h_2(\omega_m) \right) \\
\leq \quad & \frac{1}{2} \sup_{h \in \mathcal{H}} \left(u_{m-1}(h) + s\alpha h(\omega_m) \right) + \frac{1}{2} \sup_{h \in \mathcal{H}} \left(u_{m-1}(h) - s\alpha h(\omega_m) \right) \\
= \quad & \frac{1}{2} \sum_{\sigma_m \in \{-1,+1\}} \sup_{h \in \mathcal{H}} \left(u_{m-1}(h) + \alpha \sigma_m h(\omega_m) \right).
\end{aligned}
$$

Since the inequality holds for any $\epsilon > 0$, we have

$$\begin{aligned} & \frac{1}{2} \sum_{\sigma_m \in \{-1,+1\}} \sup_{h \in \mathcal{H}} \left(u_{m-1}(h) + \sigma_m (\Phi \circ h)(\omega_m)\right) \\ \leq \quad & \frac{1}{2} \sum_{\sigma_m \in \{-1,+1\}} \sup_{h \in \mathcal{H}} \left(u_{m-1}(h) + \alpha \sigma_m h(\omega_m)\right). \end{aligned}$$

Now we have

$$\begin{aligned} \hat{\mathfrak{R}}_S(\Phi \circ \mathcal{H}) \quad \leq \quad & \frac{1}{2^{m-1}} \sum_{\sigma_1, \sigma_2, \ldots, \sigma_{m-1} \in \{-1,+1\}} \frac{1}{2} \sum_{\sigma_m \in \{-1,+1\}} \frac{1}{m} \\ & \sup_{h \in \mathcal{H}} \left(\sum_{i=1}^{m-1} \sigma_i (\Phi \circ h)(\omega_i) + \alpha \sigma_m h(\omega_m) \right) \\ = \quad & \frac{1}{2^{m-1}} \sum_{\sigma_1, \ldots, \sigma_{m-2}, \sigma_m \in \{-1,+1\}} \frac{1}{2} \sum_{\sigma_{m-1} \in \{-1,+1\}} \frac{1}{m} \\ & \sup_{h \in \mathcal{H}} \left(u_{m-2}(h) + \sigma_{m-1} (\Phi \circ h)(\omega_{m-1})\right), \end{aligned}$$

where $u_{m-2}(h) \triangleq \sum_{i=1}^{m-2} \sigma_i (\Phi \circ h)(\omega_i) + \alpha \sigma_m h(\omega_m)$. Since $\sup_{h \in \mathcal{H}} \left(\sum_{i=1}^{m-1} \sigma_i (\Phi \circ h)(\omega_i) + \alpha \sigma_i h(\omega_i) \right)$ is finite for any given $\sigma_1, \sigma_2, \ldots, \sigma_m$ by assumption, by proceeding similar argument in above, we have

$$
\begin{aligned}
\hat{\mathfrak{R}}_S(\Phi \circ \mathcal{H}) &\leq \frac{1}{2^{m-1}} \sum_{\sigma_1,\ldots,\sigma_{m-2},\sigma_m \in \{-1,+1\}} \frac{1}{2} \sum_{\sigma_{m-1} \in \{-1,+1\}} \frac{1}{m} \\
&\quad \sup_{h \in \mathcal{H}} \left(u_{m-2}(h) + \alpha \sigma_{m-1} h(\omega_{m-1}) \right) \\
&= \frac{1}{2^{m-1}} \sum_{\sigma_1,\ldots,\sigma_{m-2},\sigma_m \in \{-1,+1\}} \frac{1}{2} \sum_{\sigma_{m-1} \in \{-1,+1\}} \frac{1}{m} \\
&\quad \sup_{h \in \mathcal{H}} \left(\sum_{i=1}^{m-2} \sigma_i (\Phi \circ h)(\omega_i) + \alpha \sum_{i=m-1}^{m} \sigma_i h(\omega_i) \right) \\
&= \frac{1}{2^{m-1}} \sum_{\sigma_1,\ldots,\sigma_{m-3},\sigma_{m-1}\sigma_m \in \{-1,+1\}} \frac{1}{2} \sum_{\sigma_{m-2} \in \{-1,+1\}} \frac{1}{m} \\
&\quad \sup_{h \in \mathcal{H}} \left(u_{m-3}(h) + \sigma_{m-2} (\Phi \circ h)(\omega_{m-2}) \right),
\end{aligned}
$$

where $u_{m-3}(h) \triangleq \sum_{i=1}^{m-3} \sigma_i (\Phi \circ h)(\omega_i) + \alpha \sum_{i=m-1}^{m} \sigma_i h(\omega_i)$. By continuing similar argument, we have

$$
\begin{aligned}
\hat{\mathfrak{R}}_S(\Phi \circ \mathcal{H}) &\leq \frac{1}{2^m} \sum_{\sigma_1, \sigma_2, \ldots, \sigma_m \in \{-1,+1\}} \sup_{h \in \mathcal{H}} \frac{1}{m} \alpha \sum_{i=1}^{m} \sigma_i h(\omega_i) \\
&= \alpha \hat{\mathfrak{R}}_S(\mathcal{H}).
\end{aligned}
$$

$\square$

Remarks

- By assuming that

$$\sup_{h\in\mathcal{H}}\left(\sum_{i=1}^{j}\sigma_i(\Phi\circ h)(\omega_i)+\sum_{i=j+1}^{m}\alpha\sigma_i h(\omega_i)\right)$$

  is finite for all $\sigma_i \in \{-1,+1\}, i\in[1,m]$, for all $j\in[0,m]$ and for all random samples $S=(\omega_1,\ldots,\omega_m)$ of size m and by taking average over the random sample S of size m, we have

$$\mathfrak{R}_m(\Phi\circ\mathcal{H})\le\alpha\mathfrak{R}_m(\mathcal{H}).$$

- The soft inverse limiter $\Phi_\rho(x)$ with margin $\rho>0$ is a $1/\rho$-Lipschitz function since its maximum slope is $1/\rho$.

Margin-Based Generalization Bound for Binary Classification

Theorem 4.4: Let

- $\mathscr{I}$: the input space of all possible items ω, associated with a probability space $(\mathscr{I}, \mathcal{F}, P)$.
- $c : \mathscr{I} \to \{-1, +1\}$: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- $\mathscr{Y}' \subseteq \mathbb{R}$: the output space, which is a subset of $\mathbb{R}$.
- $\mathcal{H}$: a hypothesis set of $\mathscr{Y}'$-valued measurable functions on the input space $\mathscr{I}$ such that $\sup_{h\in\mathcal{H}} |h(\omega)| < +\infty \ \forall\, \omega \in \mathscr{I}$.
- $S = (\omega_1, \omega_2, \ldots, \omega_m)$: a sample of m items drawn i.i.d. from $\mathscr{I}$ according to an unknown distribution P with labels $(c(\omega_1), c(\omega_2), \ldots, c(\omega_m))$.

- $\rho > 0$: a given confidence margin.
- $L_\rho(y', y) = \Phi_\rho(y'y) : \mathbb{R} \times \mathbb{R} \to [0, 1]$: the ρ-margin loss function.
- $g_h : \mathscr{I} \times \{-1, +1\} \to [0, 1]$: the loss function associated with h under the ρ-margin loss function L_ρ, defined as $g_h(\omega, y) \triangleq L_\rho(h(\omega), y) = \Phi_\rho(h(\omega)y)$.
- $\mathcal{G} = \{g_h \mid h \in \mathcal{H}\}$: the family of loss functions associated with hypotheses in $\mathcal{H}$ under the ρ-margin loss function L_ρ.
- $\mathscr{Z} = \mathscr{I} \times \{-1, +1\}$: the input set of loss functions g_h, associated with a probability space $(\mathscr{Z}, \tilde{\mathcal{F}}, \tilde{P})$ where $\tilde{P}$ is an extension of P from on $\mathcal{F}$ to on $\tilde{\mathcal{F}} = \mathcal{F} \times 2^{\{-1,+1\}}$.
- $\tilde{S} = ((\omega_1, c(\omega_1)), \ldots, (\omega_m, c(\omega_m)))$: the labeled sample corresponding to S.
- $\hat{A}_{\tilde{S}}(g_h) = \frac{1}{m} \sum_{i=1}^m g_h(\omega_i, c(\omega_i)) = \frac{1}{m} \sum_{i=1}^m L_\rho(h(\omega_i), c(\omega_i)) = \hat{R}_{S,\rho}(h)$, the empirical ρ-margin loss of h w.r.t. c on sample S.

- $\underset{z\sim\tilde{P}}{E}[g_h(z)] = \underset{\tilde{S}\sim\tilde{P}_m}{E}[\hat{A}_{\tilde{S}}(g_h)] = \underset{S\sim P_m}{E}[\hat{R}_{S,\rho}(h)] \geq \underset{S\sim P_m}{E}[\hat{R}_S(h)] = R(h)$.

For any $\delta > 0$, with probability at least $1-\delta$, each of the following holds for all h in $\mathcal{H}$:

$$\begin{aligned} R(h) &\leq \hat{R}_{S,\rho}(h) + \frac{2}{\rho}\mathfrak{R}_m(\mathcal{H}) + \sqrt{\frac{\ln\frac{1}{\delta}}{2m}}, \\ R(h) &\leq \hat{R}_{S,\rho}(h) + \frac{2}{\rho}\hat{\mathfrak{R}}_S(\mathcal{H}) + 3\sqrt{\frac{\ln\frac{2}{\delta}}{2m}}. \end{aligned}$$

Proof. By the Rademacher complexity bound for the family $\mathcal{G}$ in Theorem 3.1, for any $\delta > 0$, with probability at least $1-\delta$, each of the following holds for all g_h in $\mathcal{G}$:

$$\begin{aligned}
\underset{z\sim\tilde{P}}{E}[g_h(z)] &\leq \frac{1}{m}\sum_{i=1}^{m} g_h(\omega_i, c(\omega_i)) + 2\mathfrak{R}_m(\mathcal{G}) + \sqrt{\frac{\ln\frac{1}{\delta}}{2m}} \\
\underset{z\sim\tilde{P}}{E}[g_h(z)] &\leq \frac{1}{m}\sum_{i=1}^{m} g_h(\omega_i, c(\omega_i)) + 2\hat{\mathfrak{R}}_{\tilde{S}}(\mathcal{G}) + 3\sqrt{\frac{\ln\frac{2}{\delta}}{2m}}.
\end{aligned}$$

Let

$$\tilde{\mathcal{H}} \triangleq \{z = (\omega, y) \mapsto h(\omega)y \mid h \in \mathcal{H}\},$$

which is a family of $(-\mathscr{Y}' \cup \mathscr{Y}')$-valued functions on the input set $\mathscr{Z} = \mathscr{I} \times \{-1,+1\}$. It is clear that $\mathcal{G} = \Phi_\rho \circ \tilde{\mathcal{H}}$. Since Φ_ρ is a bounded $1/\rho$-Lipschitz function and $\sup_{h\in\mathcal{H}} |h(\omega)|$ is finite for all $\omega \in \mathscr{I}$, $\sup_{h\in\mathcal{H}}\left(\sum_{i=1}^{j} \sigma_i \Phi_\rho(h(\omega_i)c(\omega)) + \sum_{i=j+1}^{m} \frac{1}{\rho}\sigma_i h(\omega_i)c(\omega)\right)$ is finite for all $\sigma_i \in \{-1,+1\}, i \in [1,m]$, for all $j \in [0,m]$ and for all sample $S = (\omega_1, \ldots, \omega_m)$ of size m, we have

$$\hat{\mathfrak{R}}_{\tilde{S}}(\mathcal{G}) \leq \frac{1}{\rho}\hat{\mathfrak{R}}_{\tilde{S}}(\tilde{\mathcal{H}}) \text{ and then } \mathfrak{R}_m(\mathcal{G}) \leq \frac{1}{\rho}\mathfrak{R}_m(\tilde{\mathcal{H}})$$

by Talagrand's lemma. The empirical Rademacher complexity of $\tilde{\mathcal{H}}$ is

$$\begin{aligned}
\hat{\mathfrak{R}}_{\tilde{S}}(\tilde{\mathcal{H}}) &= \frac{1}{2^m} \sum_{\sigma_1,\sigma_2,\ldots,\sigma_m \in \{-1,+1\}} \sup_{h \in \mathcal{H}} \frac{1}{m} \sum_{i=1}^{m} \sigma_i c(\omega_i) h(\omega_i) \\
&= \frac{1}{2^m} \sum_{\sigma_1,\sigma_2,\ldots,\sigma_m \in \{-1,+1\}} \sup_{h \in \mathcal{H}} \frac{1}{m} \sum_{i=1}^{m} \sigma_i h(\omega_i) = \hat{\mathfrak{R}}_S(\mathcal{H})
\end{aligned}$$

and then $\mathfrak{R}_m(\tilde{\mathcal{H}}) = \mathfrak{R}_m(\mathcal{H})$. Now with

$$\frac{1}{m}\sum_{i=1}^{m} g_h(\omega_i, c(\omega_i)) = \hat{R}_{S,\rho}(h) \text{ and } R(h) \leq \mathop{E}_{z \sim \tilde{P}}[g_h(z)],$$

the theorem is proved. $\square$

Remarks

- The margin-based generalization bound for binary classification shows the trade-off between two terms: the larger the desired margin ρ, the smaller the middle term; however, the first term, the empirical ρ-margin loss $\hat{R}_{S,\rho}(h)$, increases as a function of ρ.

Margin-Based Generalization Bound for Linear Hypotheses on Bounded Input Space with Bounded Weight Vector

Corollary 4.1: Let

- $\mathscr{I} = \bar{B}(r; \mathbf{0}) = \{\mathbf{x} : \|\mathbf{x}\| \leq r\} \subseteq \mathbb{R}^N$: a bounded input space, associated with a probability space $(\bar{B}(r; \mathbf{0}), \mathcal{F}, P)$.
- $c : \mathscr{I} \to \{-1, +1\}$: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- $\mathcal{H} = \{\mathbf{x} \mapsto \mathbf{w} \cdot \mathbf{x} \mid \|\mathbf{w}\| \leq \Lambda\}$: the set of all linear functions with bounded weight vector.
  - It is clear that $\sup_{h \in \mathcal{H}} |h(\mathbf{x})| \leq \Lambda \|\mathbf{x}\| < +\infty \ \forall \ \mathbf{x} \in \mathscr{I}$.
- $S = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m)$: a sample of m points drawn i.i.d. from the input space $\bar{B}(r; \mathbf{0})$ according to an unknown distribution P with labels $(c(\mathbf{x}_1), c(\mathbf{x}_2), \ldots, c(\mathbf{x}_m))$.

- $\rho > 0$: a given confidence margin.
- $L_\rho(y', y) = \Phi_\rho(y'y) : \mathbb{R} \times \mathbb{R} \to [0, 1]$: the ρ-margin loss function.
- $\hat{R}_{S,\rho}(h) = \frac{1}{m} \sum_{i=1}^{m} L_\rho(h(\mathbf{x}_i), c(\mathbf{x}_i)) = \frac{1}{m} \sum_{i=1}^{m} \Phi_\rho(h(\mathbf{x}_i) c(\mathbf{x}_i))$: the empirical ρ-margin loss of a linear hypothesis h in $\mathcal{H}$ w.r.t. the concept c on the sample S.
- $R(h) = \underset{\mathbf{x} \sim P}{E}[1_{\mathrm{sgn}(h(\mathbf{x})) \neq c(\mathbf{x})}]$: the generalization error of linear hypothesis $h \in \mathcal{H}$.

For any $\delta > 0$, with probability at least $1 - \delta$, all h in $\mathcal{H}$:

$$R(h) \quad \leq \quad \hat{R}_{S,\rho}(h) + 2\sqrt{\frac{r^2 \Lambda^2 / \rho^2}{m}} + \sqrt{\frac{\ln \frac{1}{\delta}}{2m}}.$$

Proof. This is a direct consequence of Theorems 4.3 and 4.4. $\square$

Remarks

- The margin-based generalization bound for linear hypotheses does not depend directly on the dimension of the input space, but only on the margin.
- It suggests that a small generalization error can be achieved when ρ/r is large (small second term) while the empirical ρ-margin loss is relatively small (first term).
  - The latter occurs when few points are either classified incorrectly or correctly, but with margin less than ρ.
- The learning guarantee in Corollary 4.1 hinges upon the hope of a good margin value ρ: if there exists a relatively large margin value $\rho > 0$ for which the empirical ρ-margin loss is small, then a small generalization error is guaranteed by the corollary.

- This favorable margin ρ depends on the distribution: while the learning bound is distribution-independent, the existence of a good margin is in fact distribution-dependent.

Strong Justification for SVM

- For $\rho = 1$, the soft inverse limiter Φ_1 with margin 1 is upper bounded by the hinge function $x \mapsto \max(1-x, 0)$:

$$\Phi_1(x) \leq \max(1-x, 0) \;\forall\, x \in \mathbb{R}$$

and then the empirical 1-margin loss $\hat{R}_{S,\rho}(h)$ of a linear hypothesis $h(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x}$ is upper bounded by the average amount of slack penalty:

$$\begin{aligned}
\hat{R}_{S,1}(h) &= \frac{1}{m}\sum_{i=1}^{m} \Phi_1(h(\mathbf{x}_i)c(\mathbf{x}_i)) \\
&\leq \frac{1}{m}\sum_{i=1}^{m} \max(1 - c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i), 0) \\
&= \frac{1}{m}\sum_{i=1}^{m} \eta_i.
\end{aligned}$$

- The margin-based generalization bound with $\rho = 1$ implies that with probability at least $1-\delta$, for any linear function $h : \mathbf{x} \mapsto \mathbf{w} \cdot \mathbf{x}$ with $\|\mathbf{w}\| \le \Lambda$ on bounded input space $\bar{B}(r; \mathbf{0})$,

$$R(h) \quad \le \quad \frac{1}{m} \sum_{i=1}^{m} \eta_i + 2\sqrt{\frac{r^2\Lambda^2}{m}} + \sqrt{\frac{\ln \frac{1}{\delta}}{2m}},$$

  where $\eta_i = \max(1 - c(\mathbf{x}_i)(\mathbf{w} \cdot \mathbf{x}_i), 0)$ are the slack penalty over the training set.

- The objective function minimized by the SVM algorithm has precisely the form of this upper bound: the first term corresponds to the slack penalty over the training set and the second to the minimization of the $\|\mathbf{w}\|$ which is equivalent to that of $\|\mathbf{w}\|^2$.

- We have been using a parameter C in SVM to adjust the relative strength in the minimization of either term.

Searching for Large-Margin Separating Hyperplanes in High-Dimensional Space

- Since margin-based generalization bound does not directly depend on the dimension of the input space and do guarantee good generalization with a favorable margin, it suggests seeking large-margin separating hyperplanes in a very high-dimensional space.
- The next lecture provides a way of doing this, in addition to overcoming the very high cost of computation with very high-dimensional vectors as well as further generalization of SVM to nonlinear separation.