Machine Learning — Statistical Methods for Machine Learning Support Vector Machines

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The Support Vector Machine (SVM) is an algorithm for learning linear classifiers. Given a linearly separable training set $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_m, y_m) \in \mathbb{R}^d \times \{-1, 1\}$, SVM outputs the linear classifier corresponding to the unique solution $\boldsymbol{w}^* \in \mathbb{R}^d$ of the following convex optimization problem with linear constraints

$$\min_{\boldsymbol{w} \in \mathbb{R}^d} \quad \frac{1}{2} \|\boldsymbol{w}\|^2$$
s.t. $y_t \boldsymbol{w}^\top \boldsymbol{x}_t \ge 1 \quad t = 1, \dots, m.$

$$(1)$$

Geometrically, w^* corresponds to the maximum margin separating hyperplane. For every linearly separable set $(x_1, y_1), \ldots, (x_m, y_m) \in \mathbb{R}^d \times \{-1, 1\}$, the maximum margin is defined by

$$\gamma^* = \max_{\boldsymbol{u}: \|\boldsymbol{u}\|=1} \min_{t=1,\dots,m} y_t \, \boldsymbol{u}^\top \boldsymbol{x}_t$$

and the vector u^* achieving the maximum margin is the maximum margin separator.

Theorem 1. For every linearly separable set $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m) \in \mathbb{R}^d \times \{-1, 1\}$, the maximum margin separator \mathbf{u}^* satisfies $\mathbf{u}^* = \gamma^* \mathbf{w}^*$, where \mathbf{w}^* is the unique solution of (1).

PROOF. Note that u^* is the solution of the following optimization problem

$$\begin{array}{ll} \max_{\boldsymbol{u} \in \mathbb{R}^d, \, \gamma > 0} & \gamma^2 \\ \text{s.t.} & \|\boldsymbol{u}\|^2 = 1 \\ & y_t \, \boldsymbol{u}^\top \boldsymbol{x}_t \geq \gamma \quad t = 1, \dots, m. \end{array}$$

Indeed, \boldsymbol{u} maximizing the margin γ is the same \boldsymbol{u} maximizing γ^2 because the function $f(\gamma) = \gamma^2$, is monotone for $\gamma > 0$. Dividing by $\gamma > 0$ both sides of each constraint $y_t \boldsymbol{u}^\top \boldsymbol{x}_t \geq \gamma$, we obtain the equivalent constraint $y_t (\boldsymbol{u}^\top \boldsymbol{x}_t)/\gamma \geq 1$. Introducing $\boldsymbol{w} = \boldsymbol{u}/\gamma$, and noting that $\|\boldsymbol{w}\|^2 = 1/\gamma^2$ because of the constraint $\|\boldsymbol{u}\|^2 = 1$, we obtain the equivalent problem

$$\begin{array}{ll} \min_{\boldsymbol{w} \in \mathbb{R}^d, \, \gamma > 0} & \|\boldsymbol{w}\|^2 \\ \mathrm{s.t.} & \gamma^2 \, \|\boldsymbol{w}\|^2 = 1 \\ & y_t \, \boldsymbol{w}^\top \boldsymbol{x}_t \geq 1 \quad t = 1, \dots, m. \end{array}$$

Now observe that the constraint $\gamma^2 \|\boldsymbol{w}\|^2 = 1$ is redundant and can be eliminated. Indeed, for all $\boldsymbol{w} \in \mathbb{R}^d$ we can find $\gamma > 0$ such that the constraint is satisfied. Multiplying the objective function by $\frac{1}{2}$, we obtain

$$\begin{array}{ll} \min_{\boldsymbol{w} \in \mathbb{R}^d} & \frac{1}{2} \|\boldsymbol{w}\|^2 \\ \text{s.t.} & y_t \, \boldsymbol{w}^\top \boldsymbol{x}_t \geq 1 \quad t = 1, \dots, m \end{array}$$

concluding the proof.

We have thus shown the equivalence between the problem of maximizing the margin of \boldsymbol{u} while keeping the norm $\|\boldsymbol{u}\|$ constant, and the problem of minimizing the norm $\|\boldsymbol{w}\|$ while keeping the margin of \boldsymbol{w} constant.

The following result helps us compute the form of the optimal solution w^* .

Lemma 2 (Fritz John optimality condition). Consider the problem

$$\begin{array}{ll} \min_{\boldsymbol{w} \in \mathbb{R}^d} & f(\boldsymbol{w}) \\ s.t. & g_t(\boldsymbol{w}) \leq 0 \quad t = 1, \dots, m \end{array}$$

where the functions f, g_1, \ldots, g_m are all differentiable. If w_0 is an optimal solution, then there exists a nonnegative vector $\boldsymbol{\alpha} \in \mathbb{R}^m$ such that

$$\nabla f(\boldsymbol{w}_0) + \sum_{t \in I} \alpha_t \nabla g_t(\boldsymbol{w}_0) = \boldsymbol{0}$$

where $I = \{1 \le t \le m : g_t(w_0) = 0\}.$

By applying the Fritz John optimality condition to the SVM objective with $f(\boldsymbol{w}) = \frac{1}{2} \|\boldsymbol{w}\|^2$ and $g_t(\boldsymbol{w}) = 1 - y_t \, \boldsymbol{w}^\top \boldsymbol{x}_t$ we obtain

$$\boldsymbol{w}^* - \sum_{t \in I} \alpha_t y_t \, \boldsymbol{x}_t = \boldsymbol{0}$$

Hence, the optimal solution has form

$$oldsymbol{w}^* = \sum_{t \in I} lpha_t y_t oldsymbol{x}_t$$

where I denotes the set of training examples (\boldsymbol{x}_t, y_t) such that $y_t(\boldsymbol{w}^*)^{\top} \boldsymbol{x}_t = 1$. These \boldsymbol{x}_t are called **support vectors**, and are all those training points for which the margin of \boldsymbol{w}^* is exactly 1. If we removed all training examples except for the support vectors, the SVM solution would not change.

We now move on to consider the case of a training set that is not linearly separable. How should we change the SVM objective? Conside the following formulation

$$\min_{\substack{(\boldsymbol{w},\boldsymbol{\xi})\in\mathbb{R}^{d+m}\\ \text{s.t.}}} \quad \frac{\lambda}{2} \|\boldsymbol{w}\|^2 + \frac{1}{m} \sum_{t=1}^m \xi_t \\ \text{s.t.} \quad y_t \, \boldsymbol{w}^\top \boldsymbol{x}_t \ge 1 - \xi_t \quad t = 1, \dots, m \\ \xi_t \ge 0 \quad t = 1, \dots, m.$$

The components of $\boldsymbol{\xi} = (\xi_1, \dots, \xi_m)$ are called **slack variables** and measure how much each margin constraint is violated by a potential solution \boldsymbol{w} . The average of these violations is then added to the objective function. Finally, a regularization parameter $\lambda > 0$ is introduced to balance the two terms.

We now consider the constraints involving the slack variables ξ_t . That is, $\xi_t \ge 1 - y_t \boldsymbol{w}^\top \boldsymbol{x}_t$ and $\xi_t \ge 0$. In order to minimize each ξ_t , we can set

$$\xi_t = \begin{cases} 1 - y_t \, \boldsymbol{w}^\top \boldsymbol{x}_t & \text{if } y_t \, \boldsymbol{w}^\top \boldsymbol{x}_t < 1 \\ 0 & \text{otherwise.} \end{cases}$$

To see this, fix $\boldsymbol{w} \in \mathbb{R}^d$. If the constraint $y_t \boldsymbol{w}^\top \boldsymbol{x}_t \ge 1$ is satisfied by \boldsymbol{w} , then ξ_t can be set to zero. Otherwise, if the constraint is not satisfied by \boldsymbol{w} , then we set ξ_t to the smallest value such that the constraint becomes satisfied, namely $1 - y_t \boldsymbol{w}^\top \boldsymbol{x}_t$. Summarizing, $\xi_t = [1 - y_t \boldsymbol{w}^\top \boldsymbol{x}_t]_+$, which is exactly the hinge loss $h_t(\boldsymbol{w})$ of \boldsymbol{w} .

The SVM problem can then be re-formulated as $\min_{\boldsymbol{\sigma}} F(\boldsymbol{w})$, where

$$F(\boldsymbol{w}) = \frac{1}{m} \sum_{t=1}^{m} h_t(\boldsymbol{w}) + \frac{\lambda}{2} \|\boldsymbol{w}\|^2$$

We now show that, even when the training set is not linearly separable, the solution w^* belongs to the subspace defined by linear combinations of training points multiplied by their labels.

Theorem 3. The minimizer w^* of F can be written as a linear combination of y_1x_1, \ldots, y_mx_m .

PROOF. By contradiction, assume

$$\boldsymbol{w}^* = \sum_{t=1}^m \alpha_t \, y_t \, \boldsymbol{x}_t + \boldsymbol{u} \tag{2}$$

where $\boldsymbol{u} \in \mathbb{R}^d$ is the component of \boldsymbol{w}^* orthogonal to the subspace spanned by $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m$. Therefore,

$$y_t \boldsymbol{u}^\top \boldsymbol{x}_t = 0 \qquad t = 1, \dots, m.$$
(3)

Now, let $\boldsymbol{v} = \boldsymbol{w}^* - \boldsymbol{u}$. First, $\|\boldsymbol{v}\|^2 \leq \|\boldsymbol{w}^*\|^2$ because in (2) we wrote \boldsymbol{w}^* as a sum of two orthogonal components and we removed one of them, and so its length decreased. Second,

$$h_t(\boldsymbol{v}) = \left[1 - y_t \boldsymbol{v}^\top \boldsymbol{x}_t\right]_+ = \left[1 - y_t \left(\boldsymbol{w}^* - \boldsymbol{u}\right)^\top \boldsymbol{x}_t\right]_+ = \left[1 - y_t \left(\boldsymbol{w}^*\right)^\top \boldsymbol{x}_t + y_t \boldsymbol{u}^\top \boldsymbol{x}_t\right]_+ = h_t(\boldsymbol{w}^*)$$

using (3). Therefore $F(\boldsymbol{v}) \leq F(\boldsymbol{w}^*)$, contradicting the optimality of \boldsymbol{w}^* . Hence $\boldsymbol{u} = \boldsymbol{0}$ and the proof is concluded.

Note that, as in the linearly separable case, w^* generally depends on a subset of support vectors. However, unlike the linearly separable case, these support vectors also include the training points associated with positive slack variables.

We proceed by showing how F can be minimized using Online Gradient Descent (OGD). First, observe that

$$F(\boldsymbol{w}) = \frac{1}{m} \sum_{t=1}^{m} \ell_t(\boldsymbol{w})$$

where $\ell_t(\boldsymbol{w}) = h_t(\boldsymbol{w}) + \frac{\lambda}{2} \|\boldsymbol{w}\|^2$ is a strongly convex function. Indeed, $\frac{\lambda}{2} \|\boldsymbol{w}\|^2$ is λ -strongly convex, and h_t is convex (and also piecewise linear). This implies that their sum is λ -strongly convex. We can then apply the OGD algorithm for strongly convex functions to the set of losses ℓ_1, \ldots, ℓ_m . This instance of OGD, which is known as **Pegasos**, can be described as follows.

Parameters: number T of rounds, regularization coefficient $\lambda > 0$ **Input:** Training set $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_m, y_m) \in \mathbb{R}^d \times \{-1, 1\}$ Set $\boldsymbol{w}_1 = \boldsymbol{0}$ For $t = 1, \ldots, T$ 1. Draw uniformly at random an element $(\boldsymbol{x}_{Z_t}, y_{Z_t})$ from the training set 2. Set $\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - \eta_t \nabla \ell_{Z_t}(\boldsymbol{w}_t)$ Output: $\overline{\boldsymbol{w}} = \frac{1}{T} (\boldsymbol{w}_1 + \cdots + \boldsymbol{w}_T)$.

Pegasos is an example of a class of algorithms known as **stochastic gradient descent**. These are OGD-like algorithms that are run over a sequence of examples randomly drawn from the training set.

We now move on to analyze Pegasos. Let $(\boldsymbol{x}_{Z_1}, y_{Z_1}), \ldots, (\boldsymbol{x}_{Z_T}, y_{Z_T})$ the sequence of training set examples that were drawn at random in step 1 of the algorithm, and let $\ell_{Z_1}, \ldots, \ell_{Z_T}$ the corresponding sequence of loss functions. Namely, $\ell_{Z_t}(\boldsymbol{w}) = h_{Z_t}(\boldsymbol{w}) + \frac{\lambda}{2} \|\boldsymbol{w}\|^2$ where $h_{Z_t}(\boldsymbol{w}) = [1 - y_{Z_t} \boldsymbol{w}^\top \boldsymbol{x}_{Z_t}]_+$.

Let w^* be the optimal SVM solution,

$$\boldsymbol{w}^* = \operatorname*{argmin}_{\boldsymbol{w} \in \mathbb{R}^d} \left(\frac{1}{m} \sum_{t=1}^m h_t(\boldsymbol{w}) + \frac{\lambda}{2} \|\boldsymbol{w}\|^2 \right) .$$
(4)

For every realization s_1, \ldots, s_T of the random variables Z_1, \ldots, Z_T , OGD analysis for strongly convex losses immediately gives

$$\frac{1}{T}\sum_{t=1}^{T}\ell_{s_t}(\boldsymbol{w}_t) \le \frac{1}{T}\sum_{t=1}^{T}\ell_{s_t}(\boldsymbol{w}^*) + \frac{G^2}{2\lambda T}\ln(T+1)$$
(5)

where $G = \max_{t=1,...,T} \|\nabla \ell_{s_t}(\boldsymbol{w}_t)\|$ is also a random variable.

In order to show how this result can be used to bound $F(\overline{w})$, we use the following fact

$$\mathbb{E}\left[\ell_{Z_t}(\boldsymbol{w}_t) \mid Z_1, \dots, Z_{t-1}\right] = \frac{1}{m} \sum_{s=1}^m \ell_s(\boldsymbol{w}_t) = F(\boldsymbol{w}_t) .$$
(6)

In other words, conditioned on the first t-1 random draws (which determine \boldsymbol{w}_t), the expected value of $\ell_{Z_t}(\boldsymbol{w}_t)$ is equal to $F(\boldsymbol{w}_t)$. We also use the fact that for every pair of random variables

X, Y the following holds $\mathbb{E}[X] = \mathbb{E}[\mathbb{E}[X \mid Y]]$. Hence, we can write

$$\mathbb{E}[F(\overline{\boldsymbol{w}})] = \mathbb{E}\left[F\left(\frac{1}{T}\sum_{t=1}^{T}\boldsymbol{w}_{t}\right)\right]$$

$$\leq \mathbb{E}\left[\frac{1}{T}\sum_{t=1}^{T}F(\boldsymbol{w}_{t})\right] \text{ using Jensen inequality, since } F \text{ is convex}$$

$$= \mathbb{E}\left[\frac{1}{T}\sum_{t=1}^{T}\mathbb{E}[\ell_{Z_{t}}(\boldsymbol{w}_{t}) \mid Z_{1}, \dots, Z_{t-1}]\right] \text{ using } (6)$$

$$= \mathbb{E}\left[\frac{1}{T}\sum_{t=1}^{T}\ell_{Z_{t}}(\boldsymbol{w}_{t})\right] \text{ using } \mathbb{E}[X] = \mathbb{E}[\mathbb{E}[X \mid Y]]$$

$$\leq \mathbb{E}\left[\frac{1}{T}\sum_{t=1}^{T}\ell_{Z_{t}}(\boldsymbol{w}^{*})\right] + \frac{\mathbb{E}[G^{2}]}{2\lambda T}(\ln T + 1) \text{ using } (5)$$

$$= \mathbb{E}\left[\frac{1}{T}\sum_{t=1}^{T}\mathbb{E}[\ell_{Z_{t}}(\boldsymbol{w}^{*}) \mid Z_{1}, \dots, Z_{t-1}]\right] + \frac{\mathbb{E}[G^{2}]}{2\lambda T}(\ln T + 1) \text{ using } \mathbb{E}[X] = \mathbb{E}[\mathbb{E}[X \mid Y]]$$

$$= F(\boldsymbol{w}^{*}) + \frac{\mathbb{E}[G^{2}]}{2\lambda T}\ln(T + 1) \text{ using } (6).$$

We thus obtained

$$\mathbb{E}\left[F(\overline{\boldsymbol{w}})\right] \le F(\boldsymbol{w}^*) + \frac{\mathbb{E}\left[G^2\right]}{2\lambda T} \left(\ln T + 1\right) \,. \tag{7}$$

Therefore, if $\mathbb{E}[G^2]$ can be upper bounded by a constant, the average \overline{w} of the vectors generated by OGD converges (in expectation with respect to the random draw of the elements from the training set) to w^* with rate $\frac{\ln T}{T}$. With a bit more work, one can show that \overline{w} converges to w^* not only in expectation but also in probability.

We now bound G for every realization s_1, \ldots, s_T of the random variables Z_1, \ldots, Z_T . We have $\nabla \ell_{s_t}(\boldsymbol{w}_t) = -y_{s_t} \boldsymbol{x}_{s_t} \mathbb{I}\{h_{s_t}(\boldsymbol{w}_t) > 0\} + \lambda \boldsymbol{w}_t$. Let $\boldsymbol{v}_t = y_{s_t} \boldsymbol{x}_{s_t} \mathbb{I}\{h_{s_t}(\boldsymbol{w}_t) > 0\}$. Because $\eta_t = 1/(\lambda t)$, the update rule for \boldsymbol{w}_t takes the following simple form,

$$oldsymbol{w}_{t+1} = oldsymbol{w}_t - \eta_t
abla \ell_t(oldsymbol{w}_t) = oldsymbol{w}_t + \eta_t oldsymbol{v}_t - \eta_t \lambda oldsymbol{w}_t = \left(1 - rac{1}{t}
ight) oldsymbol{w}_t + rac{1}{\lambda t} oldsymbol{v}_t \; .$$

Let $X = \max_{s=1,...,m} \|\boldsymbol{x}_s\|$. Since $\|\nabla \ell_{s_t}(\boldsymbol{w}_t)\| \leq \|\boldsymbol{v}_t\| + \lambda \|\boldsymbol{w}_t\| \leq X + \lambda \|\boldsymbol{w}_t\|$, we are left with the task of computing an upper bound for $\|\boldsymbol{w}_t\|$. In order to do so, we look at the recurrence

$$oldsymbol{w}_{t+1} = \left(1-rac{1}{t}
ight)oldsymbol{w}_t + rac{1}{\lambda t}oldsymbol{v}_t \; .$$

As one can easily show by induction, \boldsymbol{w}_{t+1} can be written as a linear combination of $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_t$. In order to determine the coefficients of this linear combination, we fix $s \leq t$ and observe that \boldsymbol{v}_s is added to the sum with coefficient $1/(\lambda s)$. When \boldsymbol{w}_{t+1} , is computed, the coefficient of \boldsymbol{v}_s has become

$$\frac{1}{\lambda s} \prod_{r=s+1}^{t} \left(1 - \frac{1}{r} \right) = \frac{1}{\lambda s} \prod_{r=s+1}^{t} \frac{r-1}{r} = \frac{1}{\lambda t} \ .$$

We thus obtain a simple expression for w_{t+1} ,

$$\boldsymbol{w}_{t+1} = \frac{1}{\lambda t} \sum_{s=1}^{t} \boldsymbol{v}_s \;. \tag{8}$$

Because \boldsymbol{w}_{t+1} is an average of \boldsymbol{v}_s divided by λ , we finally have $\|\boldsymbol{w}_{t+1}\| \leq \frac{1}{\lambda} \max_s \|\boldsymbol{v}_s\| \leq \frac{1}{\lambda} X$. This allows us to conclude that $\|\nabla \ell_t(\boldsymbol{w}_t)\| \leq X + \lambda \|\boldsymbol{w}_t\| \leq 2X$. Substituting this bound for G in (7) we get

$$\mathbb{E}[F(\overline{\boldsymbol{w}})] \le F(\boldsymbol{w}^*) + \frac{2X^2}{\lambda T} \ln(T+1)$$

Theorem 3 states that the solution w^* to the SVM problem can be written as

$$\boldsymbol{w}^* = \sum_{s \in S} y_s \alpha_s \boldsymbol{x}_s$$

where $\alpha_s > 0$ and $S \equiv \{t = 1, ..., m : h_t(\boldsymbol{w}^*) > 0\}$. An important consequence of this result is that we can solve the problem (4) in a RKHS \mathcal{H}_K , where the objective function F becomes

$$F_K(g) = \frac{1}{m} \sum_{t=1}^m h_t(g) + \frac{\lambda}{2} \|g\|_K^2 \qquad g \in \mathcal{H}_K$$

with $h_t(g) = [1 - y_t g(\boldsymbol{x}_t)]_+$. In \mathcal{H}_K , the SVM solution can therefore be written as

$$\sum_{s\in S} y_s \alpha_s K(\boldsymbol{x}_s, \cdot)$$

which is clearly an element of the RKHS

$$\mathcal{H}_K \equiv \left\{ \sum_{i=1}^N \alpha_i \, K(\boldsymbol{x}_i, \cdot) \, : \, \boldsymbol{x}_1, \dots, \boldsymbol{x}_N \in \mathbb{R}^d, \, \alpha_1, \dots, \alpha_N \in \mathbb{R}, \, N \in \mathbb{N} \right\}$$

As we did for the Perceptron, we can run Pegasos in the RKHS \mathcal{H}_K . The gradient update in kernel Pegasos on some training example $(\boldsymbol{x}_{s_t}, y_{s_t})$ can be written as

$$g_{t+1} = \left(1 - \frac{1}{t}\right)g_t + \frac{y_{s_t}}{\lambda t} \mathbb{I}\{h_{s_t}(g_t) > 0\} K(\boldsymbol{x}_{s_t}, \cdot)$$

where $h_{s_t}(g_t) = [1 - y_{s_t}g_t(\boldsymbol{x}_{s_t})]_+$.