Support Vector Classifiers in `scikit-learn`: Mathematical Detail, Part I

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Abstract

We present the mathematical detail pertaining to the theory of support vector classifiers, focusing our attention on hard-margin linear classifiers. We describe the rationale behind support vector classifiers, and provide extensive foundational detail. We construct the primal problem and, subsequently, derive the dual problem. We also show how the primal problem can be derived from the dual problem. The paper is the first in a series, and is intended to be educational in nature.

1 Introduction

The support vector classifier (SVC) library in `scikit-learn` is used for classification of labelled data. In this paper, and others to follow, we intend to describe, in detail, the underlying mathematics of the principal algorithms in this library. Here, we will discuss relevant introductory ideas and hard-margin SVCs, considering the formulation of both the primal and dual problems. In future work we will define and discuss the soft-margin classifiers C-SVC and ν-SVC.

2 Support Vector Classifier rationale

Here is a brief list describing, in broad terms, the rationale behind support vector classifiers. Of course, the notes that follow will contain significantly more detail, but this list should serve as a good starting point.

- Assume we have a dataset X comprising two classes S_- and S_+. Each data point $\mathbf{x}_i \in X$ is an *M*-dimensional real-valued vector $\left(\mathbf{x}_i \in \mathbb{R}^M\right)$. This *M*-dimensional space is termed the input space.
- We assume that the dataset has been suitably preprocessed, in the sense that outliers have been removed and that each component of the data points has been normalized in such a way that each data point lies in the unit hypercube $\left[0,1\right]^M$.
- Each data point $\mathbf{x}_i$ carries a *label* y_i. We use $y_i = -1$ for class S_- and $y_i = +1$ for class S_+.
- We seek to find a *hyperplane* in the *M*-dimensional input space such that the hyperplane separates the two classes. Ideally, all data points in S_- will lie on one side of the hyperplane, and all data points in S_+ will lie on the other side of the hyperplane.
- This hyperplane is known as the *decision surface*. When a *test point* $\mathbf{z}$ is to be classified as either an element of S_- or S_+, its *discriminant* is determined. The discriminant is related to the signed distance of $\mathbf{z}$ from the decision surface. The sign of the

discriminant determines the label assigned to $\mathbf{z}$. The set of test points Z can be labelled or unlabelled. If it is labelled, then it is used as a test of the quality of the classifier. If it is unlabelled, then it constitutes the very input for which the classifier is designed.

- Our approach is, in fact, to find two distinct *parallel* hyperplanes, each of which separates the data, such that the perpendicular distance between these two hyperplanes is *maximal* (see the last point in this list). The decision surface is then simply the average, or midpoint, of these two parallel hyperplanes.
- The region between the two parallel hyperplanes is known as the *separating margin* or, simply, the *margin*.
- Because the margin width is maximal, the decision surface is deemed to be optimal, since it separates the two classes *as much as possible*.
- An *M*-dimensional hyperplane is described using $M+1$ coefficients. Hence, finding the decision surface is clearly a multidimensional optimization problem.
- The preceding points describe the rationale behind the construction of an SVC with a so-called *linear kernel*. In a later paper, we will extend our analysis to include nonlinear kernels, which may operate in infinite-dimensional spaces. In fact, it is possible to construct an SVC without explicitly determining the decision surface, and this is the favoured approach with nonlinear kernels. Indeed, in such cases we determine the discriminant directly.

- The idea of seeking a margin of maximal width is certainly intuitive, but it is also principled: for a given dataset X, the **Vapnik-Chervonenkis (VC) dimension** of an SVC for this set indicates the *capacity* or *capability* of the SVC to properly classify the data points of the set. It turns out that this VC dimension is inversely proportional to the margin width. Moreover, it is known that to minimize the *structural risk* (a measure of how simple or how complex the SVC should be, and where a minimal value is considered optimal), we should choose the SVC that has *minimal* VC dimension, i.e. the SVC with maximal margin width. In practice, we do not calculate the VC dimension for our datasets, and we will not encounter the VC dimension again in this paper, but this brief discussion shows that choosing the SVC with maximal margin width is not merely sensible, but also theoretically meaningful.

3 Hyperplane concepts

In this section we list a variety of mathematical concepts relevant to hyperplanes in $\mathbb{R}^M$. All of these ideas will be of significance in this paper.

Assume the notation $\mathbf{v} = (v_1, v_2, \ldots, v_M)$, $\mathbf{x} = (x_1, x_2, \ldots, x_M)$, $\mathbf{x}_i = (x_{i,1}, x_{i,2}, \ldots, x_{i,M})$. These are vectors in $\mathbb{R}^M$. The components of $\mathbf{x}$ denote the coordinates in $\mathbb{R}^M$.

Let two hyperplanes be denoted by $P_1(\mathbf{x}) = \mathbf{v} \cdot \mathbf{x} + c_1 = 0$ and $P_2(\mathbf{x}) = \mathbf{v} \cdot \mathbf{x} + c_2 = 0$.

The gradient of $P_1(\mathbf{x})$ is given by

$$\nabla P_1(\mathbf{x}) = \left(\frac{\partial P_1}{\partial x_1}, \frac{\partial P_1}{\partial x_2}, \ldots, \frac{\partial P_1}{\partial x_N} \right) = (v_1, v_2, \ldots, v_N) = \mathbf{v}$$

and similarly for $P_2(\mathbf{x})$. Since these hyperplanes have the same gradient, they are parallel. Moreover, $\mathbf{v} \perp P_1, P_2$.

Let $\mathbf{x}_1$ be a point on $P_1(\mathbf{x})$. Hence, $\mathbf{v} \cdot \mathbf{x}_1 + c_1 = 0$. Let $\mathbf{x}_2$ be a point on $P_2(\mathbf{x})$ such that $\mathbf{x}_2 = \mathbf{x}_1 + \delta \hat{\mathbf{v}}$, where $\hat{\mathbf{v}}$ is the unit vector of $\mathbf{v}$, and $\delta \in \mathbb{R}$. This statement means that $\mathbf{x}_2$, which is on P_2, is *perpendicularly opposite* to $\mathbf{x}_1$. The perpendicular distance D from $\mathbf{x}_1$ to $\mathbf{x}_2$ is $D = |\delta| = \sqrt{\delta \cdot \delta}$.

Now, using $\mathbf{v} \cdot \mathbf{v} = |\mathbf{v}|^2$ and $\hat{\mathbf{v}} = \mathbf{v}/|\mathbf{v}| = \mathbf{v}/\sqrt{\mathbf{v} \cdot \mathbf{v}}$, we have

$$\begin{aligned} \mathbf{v} \cdot \mathbf{x}_2 &= \mathbf{v} \cdot \mathbf{x}_1 + \delta \mathbf{v} \cdot \hat{\mathbf{v}} = \mathbf{v} \cdot \mathbf{x}_1 + \delta \frac{\mathbf{v} \cdot \mathbf{v}}{\sqrt{\mathbf{v} \cdot \mathbf{v}}} \\ &= \mathbf{v} \cdot \mathbf{x}_1 + \delta |\mathbf{v}|. \end{aligned}$$

Since $\mathbf{x}_2$ is on P_2, we have $\mathbf{v} \cdot \mathbf{x}_2 + c_2 = 0$, and so

$$\begin{aligned} &-c_2 = -c_1 + \delta |\mathbf{v}| \\ &\Rightarrow \delta = \frac{c_1 - c_2}{|\mathbf{v}|} \Rightarrow D = |\delta| = \frac{|c_1 - c_2|}{|\mathbf{v}|}. \end{aligned}$$

The average or *midpoint* of the two hyperplanes is

$$P_0(\mathbf{x}) = \frac{2\mathbf{v}\cdot\mathbf{x}+c_1+c_2}{2}$$
$$= \mathbf{v}\cdot\mathbf{x}+\frac{c_1+c_2}{2} = 0.$$

Now, consider two hyperplanes given by

$$\mathbf{v}\cdot\mathbf{x}+a=+\rho$$
$$\mathbf{v}\cdot\mathbf{x}+a=-\rho$$

where $\rho>0.$ Rewriting these as

$$\mathbf{v}\cdot\mathbf{x}+a-\rho=0$$
$$\mathbf{v}\cdot\mathbf{x}+a+\rho=0$$

and defining

$$c_1=a+\rho$$
$$c_2=a-\rho$$

gives

$$D=|\delta|=\left|\frac{a+\rho-(a-\rho)}{|\mathbf{v}|}\right|=\frac{2\rho}{|\mathbf{v}|}.$$

Note that if $\rho=1,\ D=2/|\mathbf{v}|.$

The midpoint hyperplane is given by

$$\frac{2\mathbf{v}\cdot\mathbf{x}+c_1+c_2}{2}=\mathbf{v}\cdot\mathbf{x}+\frac{a+\rho+a-\rho}{2}$$
$$=\mathbf{v}\cdot\mathbf{x}+a=0.$$

Lastly, the *signed* distance $\bar{\Delta}$ from an arbitrary test point $\mathbf{z} = (z_1, z_2, \ldots, z_M)$ to the hyperplane $\mathbf{v} \cdot \mathbf{x} + a = 0$ is given by

$$\bar{\Delta}(\mathbf{z}|\mathbf{v}, a) = \frac{\mathbf{v} \cdot \mathbf{z} + a}{|\mathbf{v}|} = \frac{\Delta(\mathbf{z}|\mathbf{v}, a)}{|\mathbf{v}|}$$

where we have implicitly defined the *discriminant* $\Delta(\mathbf{z}|\mathbf{v}, a) = \mathbf{v} \cdot \mathbf{z} + a$. The signed distance is a very important concept in SVCs. If the hyperplane $\mathbf{v} \cdot \mathbf{x} + a = 0$ is the decision surface of an SVC, then it is the sign of $\bar{\Delta}(\mathbf{z}|\mathbf{v}, a)$ (or, equivalently, $\Delta(\mathbf{z}|\mathbf{v}, a)$) that determines the classification of the test point $\mathbf{z}$ by that SVC.

4 The SVC optimization problem

Let us return to the two classes of data S_- and S_+. We assume that we have a dataset (the so-called *training* set) $X = \{(\mathbf{x}_i, y_i)\}_{i=1}^{N}$ of labelled data points, and $X = S_- \bigcup S_+$. We assume that the dataset has been suitably preprocessed.

We define two hyperplanes $\mathbf{v} \cdot \mathbf{x} + a = \rho$ and $\mathbf{v} \cdot \mathbf{x} + a = -\rho$. We demand that all data points $\mathbf{x}_i$ with $y_i = -1$ lie 'below' the hyperplane $\mathbf{v} \cdot \mathbf{x} + a = -\rho$, i.e. $\mathbf{v} \cdot \mathbf{x}_i + a \le -\rho$ when $y_i = -1$.

Similarly, we demand that all data points $\mathbf{x}_i$ with $y_i = +1$ lie 'above' the hyperplane $\mathbf{v} \cdot \mathbf{x} + a = \rho$, i.e. $\mathbf{v} \cdot \mathbf{x}_i + a \ge \rho$ when $y_i = +1$.

These conditions can be combined as

$$y_i(\mathbf{v}\cdot\mathbf{x}_i + a) \geq \rho .$$

Obviously, when $y_i = +1$ we find $\mathbf{v}\cdot\mathbf{x}_i + a \geq \rho$, and when $y_i = -1$ we find $-(\mathbf{v}\cdot\mathbf{x}_i + a) \geq \rho \Rightarrow \mathbf{v}\cdot\mathbf{x}_i + a \leq -\rho$. Note that we could write this expression as $y_i\, \Delta(\mathbf{x}_i | \mathbf{v}, a) \geq \rho$, but this notation is not widely used.

The two hyperplanes $\mathbf{v}\cdot\mathbf{x} + a = \rho$ and $\mathbf{v}\cdot\mathbf{x} + a = -\rho$ define the margin, which has width $D = 2\rho / |\mathbf{v}|$. Clearly, D can be maximized if $|\mathbf{v}| = \sqrt{\mathbf{v}\cdot\mathbf{v}}$ is minimized. Moreover, if $\frac{\mathbf{v}\cdot\mathbf{v}}{2}$ is minimized, then $|\mathbf{v}|$ is also minimized. The decision surface is the midpoint of the two hyperplanes and is given by $\mathbf{v}\cdot\mathbf{x} + a = 0$.

Hence, the traditional problem statement for an SVC is:

Given the training set $\{(\mathbf{x}_i, y_i)\}_{i=1}^{N}$ and $\rho > 0$, find the values of $\mathbf{v}$ and a such that

$$F_p(\mathbf{v}) = \frac{\mathbf{v}\cdot\mathbf{v}}{2}$$

is minimized, and the constraints

$$y_i(\mathbf{v}\cdot\mathbf{x}_i + a) \geq \rho$$

are satisfied, for $i = 1, 2, \ldots, N$.

This is known as the **primal** problem. The minimization of $F_p(\mathbf{v})$ necessarily means that $|\mathbf{v}|$ is minimized, and so the width of the margin D is maximized. If we divide by ρ we find $y_i\left(\frac{\mathbf{v}}{\rho}\cdot\mathbf{x}_i+\frac{a}{\rho}\right)\geq\frac{\rho}{\rho}=1$ and $F_p(\mathbf{v})=\frac{\rho^2}{2}\left(\frac{\mathbf{v}}{\rho}\cdot\frac{\mathbf{v}}{\rho}\right)$, and if we relabel according to $\mathbf{w}=\mathbf{v}/\rho$, $b=a/\rho$, we find $y_i(\mathbf{w}\cdot\mathbf{x}_i+b)\geq 1$, $F_p(\mathbf{w})=\rho^2\left(\frac{\mathbf{w}\cdot\mathbf{w}}{2}\right)$ and, obviously, the $\mathbf{w}$ that minimizes $\rho^2\left(\frac{\mathbf{w}\cdot\mathbf{w}}{2}\right)$ is the same $\mathbf{w}$ that minimizes $\frac{\mathbf{w}\cdot\mathbf{w}}{2}$.

Hence, we may restate the primal problem as:

Given the training set $\{(\mathbf{x}_i, y_i)\}_{i=1}^{N}$, find the values of $\mathbf{w}$ and b such that

$$F_p(\mathbf{w})=\frac{\mathbf{w}\cdot\mathbf{w}}{2}$$

is minimized, and the constraints

$$y_i(\mathbf{w}\cdot\mathbf{x}_i+b)\geq 1$$

are satisfied, for $i=1,2,\ldots,N$.

In this form, the primal problem does not contain the parameter ρ, and the margin has width $D = 2/|\mathbf{w}|$. In a later section, we will encounter a type of SVC in which ρ is a parameter to be determined, rather than given. The decision surface is given by $\mathbf{w}\cdot\mathbf{x} + b = 0$.

The primal problem is a minimization problem with inequality constraints. To solve it, we must write down the Karusch-Kuhn-Tucker (KKT) conditions

$$L(\mathbf{w},b,\alpha) = \frac{\mathbf{w}\cdot\mathbf{w}}{2} - \sum_{i=1}^{N}\alpha_i\left[y_i\left(\mathbf{w}\cdot\mathbf{x}_i + b\right) - 1\right]$$

$$\left.\begin{array}{c} \frac{\partial L}{\partial \mathbf{w}} = 0, \ \frac{\partial L}{\partial b} = 0 \\ \alpha_i\left[y_i\left(\mathbf{w}\cdot\mathbf{x}_i + b\right) - 1\right] = 0, \ \alpha_i \geq 0 \\ y_i\left(\mathbf{w}\cdot\mathbf{x}_i + b\right) - 1 \geq 0 \end{array}\right\} \text{KKT conditions}$$

The function $L(\mathbf{w},b,\alpha)$ is known as the **Lagrangian**, and the factors α_i are the *KKT multipliers*. The expressions highlighted in blue are the *stationarity* conditions, and the equations in red are known as the *complementarity* conditions. The inequalities in green font will be referred to as the *feasibility* conditions.

Essentially, we find the optimal solution by solving the stationarity conditions, subject to restrictions imposed by the complementarity conditions. The solution must satisfy the feasibility conditions which in turn, can sometimes be helpful in obtaining the solution. We will see this process in action in a later section, where we will solve one or two simple cases in detail.

It is possible to use the KKT conditions to reconstruct the primal problem in a particularly useful way. We have

$$\frac{\partial L}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{w} - \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i = 0 \Rightarrow \mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$$

$$\frac{\partial L}{\partial b} = 0 \Rightarrow \sum_{i=1}^{N} \alpha_i y_i = 0.$$

Expanding the Lagrangian gives

$$L(\mathbf{w}, b, \alpha) = \frac{\mathbf{w} \cdot \mathbf{w}}{2} - \sum_{i=1}^{N} \alpha_i y_i \mathbf{w} \cdot \mathbf{x}_i - b \sum_{i=1}^{N} \alpha_i y_i + \sum_{i=1}^{N} \alpha_i.$$

We also have

$$\sum_{i=1}^{N} \alpha_i y_i \mathbf{w} \cdot \mathbf{x}_i = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i \cdot \mathbf{w} = \mathbf{w} \cdot \mathbf{w}$$

and so

$$\begin{aligned} L(\alpha) &= \frac{\mathbf{w} \cdot \mathbf{w}}{2} - \mathbf{w} \cdot \mathbf{w} - 0 + \sum_{i=1}^{N} \alpha_i = -\frac{\mathbf{w} \cdot \mathbf{w}}{2} + \sum_{i=1}^{N} \alpha_i \\ &= -\frac{1}{2} \left(\sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i \right) \cdot \left(\sum_{j=1}^{N} \alpha_j y_j \mathbf{x}_j \right) + \sum_{i=1}^{N} \alpha_i \\ &= -\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j + \sum_{i=1}^{N} \alpha_i. \end{aligned}$$

From optimization theory, we know that maximizing this expression with respect to α is equivalent to solving the primal problem. However, it is traditional to express SVC optimization as a minimization problem, and so we actually seek to minimize $-L(\alpha)$.

This is known as the **dual** problem, and we state it as

Given the training set $\left\{\left(\mathbf{x}_i, y_i\right)\right\}_{i=1}^{N}$, find the values of $\left\{\alpha_i\right\}_{i=1}^{N}$ such that

$$F_d\left(\alpha\right) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j - \sum_{i=1}^{N}\alpha_i$$

is minimized, and the constraints

$$\alpha_i \geq 0 \quad \text{for } i = 1, 2, \ldots, N$$
$$\sum_{i=1}^{N}\alpha_i y_i = 0$$

are satisfied.

Two significant observations can be made: (1) the only unknowns in the problem are the KKT multipliers α_i, and (2) the data points appear in the problem only in the form of the scalar product $\mathbf{x}_i \cdot \mathbf{x}_j$. This second observation will be seen to be extremely important when we deal with nonlinear classifiers. We remind ourselves that, once the dual problem is solved, and the α_i are known, we find $\mathbf{w}$ from $\mathbf{w} = \sum_{i=1}^{N}\alpha_i y_i \mathbf{x}_i$, which was derived previously from one of the stationarity conditions. It is this expression for $\mathbf{w}$ that gives SVCs their name – only nonzero values of α_i can make a contribution to the sum, and the corresponding $\mathbf{x}_i$ are known as **support vectors**.

The calculation of the intercept b utilises the complementarity condition. For each support vector $\alpha_i \neq 0$. Hence, for the complementarity condition to be satisfied, we must have $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1 = 0$. This gives

$$\begin{aligned} & y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1 = 0 \\ \Rightarrow\ & \mathbf{w} \cdot \mathbf{x}_i + b - y_i = 0 \\ \Rightarrow\ & b = y_i - \mathbf{w} \cdot \mathbf{x}_i = y_i - \sum_{j=1}^{N} y_j \alpha_j \mathbf{x}_j \cdot \mathbf{x}_i. \end{aligned}$$

For numerical stability we take the average value over all support vectors

$$b = \frac{1}{N_\Omega} \sum_{\mathbf{x}_i \in \Omega} \left(y_i - \sum_{j=1}^{N} y_j \alpha_j \mathbf{x}_j \cdot \mathbf{x}_i \right)$$

where Ω is the set of all support vectors, and N_Ω is the cardinality of the set Ω.

5 Deriving the primal from the dual

Just as the dual problem is derived from the primal problem, so the primal problem can be derived from the dual, with a suitable choice of Lagrange and KKT multipliers.

A useful derivative

Before we proceed, it will be useful to differentiate the function

$$F_d(\alpha) = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j - \sum_{i=1}^{N} \alpha_i$$

$$= \frac{1}{2}\sum_{k=1}^{N}\sum_{j=1}^{N}\alpha_k\alpha_j y_k y_j \mathbf{x}_k \cdot \mathbf{x}_j - \sum_{k=1}^{N}\alpha_k$$

where we have replaced the sum over *i* with a sum over *k*, for notational convenience.

We seek the derivative of this function with respect to α_i. So, we have

$$\begin{aligned}
\frac{\partial F_d}{\partial \alpha_i} &= \frac{1}{2}\sum_{k=1}^{N}\sum_{j=1}^{N} y_k y_j \mathbf{x}_k \cdot \mathbf{x}_j \frac{\partial \alpha_k \alpha_j}{\partial \alpha_i} - \sum_{k=1}^{N}\frac{\partial \alpha_k}{\partial \alpha_i} \\
&= \frac{1}{2}\sum_{k=1}^{N}\sum_{j=1}^{N} y_k y_j \mathbf{x}_k \cdot \mathbf{x}_j \left(\alpha_k \frac{\partial \alpha_j}{\partial \alpha_i} + \alpha_j \frac{\partial \alpha_k}{\partial \alpha_i}\right) - \sum_{k=1}^{N}\frac{\partial \alpha_k}{\partial \alpha_i} \\
&= \frac{1}{2}\sum_{k=1}^{N}\sum_{j=1}^{N} y_k y_j \mathbf{x}_k \cdot \mathbf{x}_j \left(\alpha_k \delta_{ji} + \alpha_j \delta_{ki}\right) - \sum_{k=1}^{N}\delta_{ki} \\
&= \frac{1}{2}\sum_{k=1}^{N}\sum_{j=1}^{N} y_k y_j \mathbf{x}_k \cdot \mathbf{x}_j \alpha_k \delta_{ji} + \frac{1}{2}\sum_{k=1}^{N}\sum_{j=1}^{N} y_k y_j \mathbf{x}_k \cdot \mathbf{x}_j \alpha_j \delta_{ki} - \sum_{k=1}^{N}\delta_{ki}.
\end{aligned}$$

Consider the first sum. Since $\delta_{ij} = 1$ when $i = j$, and $\delta_{ij} = 0$ when $i \neq j$, we have

$$\sum_{j=1}^{N} y_k y_j \mathbf{x}_k \cdot \mathbf{x}_j \alpha_k \delta_{ji} = 0 + 0 + \ldots + y_k y_i \mathbf{x}_k \cdot \mathbf{x}_i \alpha_k + \ldots + 0$$

so that

$$\begin{aligned}
\frac{1}{2}\sum_{k=1}^{N}\sum_{j=1}^{N} y_k y_j \mathbf{x}_k \cdot \mathbf{x}_j \alpha_k \delta_{ji} &= \frac{1}{2}\sum_{k=1}^{N} y_k y_i \mathbf{x}_k \cdot \mathbf{x}_i \alpha_k \\
&= \frac{1}{2}\sum_{j=1}^{N} y_j y_i \mathbf{x}_j \cdot \mathbf{x}_i \alpha_j
\end{aligned}$$

where we have replaced the index *k* with *j*.

The second sum becomes

$$\frac{1}{2}\sum_{k=1}^{N}\sum_{j=1}^{N} y_k y_j \mathbf{x}_k \cdot \mathbf{x}_j \alpha_j \delta_{ki} = \frac{1}{2}\sum_{j=1}^{N} y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j \alpha_j$$

using $\delta_{ki} = 1$ when $k = i$, and $\delta_{ki} = 0$ when $k \neq i$. Clearly, these sums are equal.

The third sum is simply

$$\sum_{k=1}^{N} \delta_{ki} = 0 + 0 + \ldots + \delta_{ii} + \ldots + 0 = 1.$$

Hence,

$$\begin{aligned}\frac{\partial F_d}{\partial \alpha_i} &= \frac{1}{2}\sum_{j=1}^{N} y_j y_i \mathbf{x}_j \cdot \mathbf{x}_i \alpha_j + \frac{1}{2}\sum_{j=1}^{N} y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j \alpha_j - 1 \\ &= y_i \sum_{j=1}^{N} \alpha_j y_j \mathbf{x}_j \cdot \mathbf{x}_i - 1\end{aligned}$$

where we have factored y_i out of the sum, since it is independent of j.

The hard-margin classifier

For the hard-margin classifier we have

$$F_d(\alpha) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j - \sum_{i=1}^{N} \alpha_i$$

and the constraints

$$\alpha_i \geq 0 \qquad \sum_{i=1}^{N} \alpha_i y_i = 0.$$

The corresponding Lagrangian is

$$L(\alpha, b, \mu) = F_d + b\sum_{i=1}^{N} y_i \alpha_i - \sum_{i=1}^{N} \mu_i \alpha_i$$

where b and $\mu_i \geq 0$ are appropriate multipliers. The Lagrange multiplier b can be of any sign since it corresponds to an equality condition. Stationarity gives

$$\frac{\partial L}{\partial \alpha_i} = \frac{\partial F_d}{\partial \alpha_i} + by_i - \mu_i = y_i \sum_{j=1}^{N} \alpha_j y_i \mathbf{x}_j \cdot \mathbf{x}_i - 1 + by_i - \mu_i = 0$$

$$\Rightarrow y_i \sum_{j=1}^{N} \alpha_j y_i \mathbf{x}_j \cdot \mathbf{x}_i = 1 - by_i + \mu_i.$$

Using the familiar expression for $\mathbf{w}$ gives

$$\begin{aligned} y_i \sum_{j=1}^{N} \alpha_j y_i \mathbf{x}_j \cdot \mathbf{x}_i &= 1 - by_i + \mu_i \\ \Rightarrow y_i \mathbf{w} \cdot \mathbf{x}_i &= 1 - by_i + \mu_i \\ \Rightarrow y_i \left(\mathbf{w} \cdot \mathbf{x}_i + b \right) &= 1 + \mu_i \\ \Rightarrow y_i \left(\mathbf{w} \cdot \mathbf{x}_i + b \right) &\geq 1 \end{aligned}$$

where we have used $\mu_i \geq 0$ in the last line. This, of course, is the set of conditions imposed in the primal problem.

To derive $F_p(\mathbf{w})$, consider the Lagrangian

$$\begin{aligned} L(\alpha, b, \mu) &= \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j - \sum_{i=1}^{N} \alpha_i + b \sum_{i=1}^{N} y_i \alpha_i - \sum_{i=1}^{N} \mu_i \alpha_i \\ &= \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j - \sum_{i=1}^{N} \alpha_i \left(1 - by_i + \mu_i \right) \\ &= \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j - \sum_{i=1}^{N} \alpha_i y_i \sum_{j=1}^{N} \alpha_j y_j \mathbf{x}_j \cdot \mathbf{x}_i \\ &= \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j - \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_j \cdot \mathbf{x}_i \\ &= -\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j. \end{aligned}$$

Since the dual is a minimization problem, this is the function that must be *maximized*. We prefer to present the primal problem as a minimization problem, though, and so we actually seek to minimize

$$F_p(\mathbf{w}) = -L(\alpha) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j = \frac{\mathbf{w}\cdot\mathbf{w}}{2}$$

subject, of course, to the conditions $y_i(\mathbf{w}\cdot\mathbf{x}_i + b) \geq 1$. Thus, we have derived the primal problem from the dual problem.

6 Concluding comments

We have described the hard-margin SVC in detail. This is foundational knowledge necessary for the next paper in this series, wherein we will discuss the soft-margin classifier, known as *C*-SVC, and implemented in **`scikit-learn`** as `svm.SVC`.

Bibliography

Rather than making use of in-text references, we provide a potentially useful bibliography. Naturally, any text pertaining to SVCs is meaningful, and we are sure our readers are well capable of conducting their own search for such resources. Nevertheless, the following list (mostly books, a few articles), although not exhaustive, is certainly representative.

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