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

J.S.C. Prentice

Senior Research Officer
Mathsophical Ltd.
Johannesburg, South Africa
jpmsro@mathsophical.com

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Abstract

We present mathematical detail pertaining to the theory of soft-margin support vector classifiers, designated C-SVC, as used in `scikit-learn`. We discuss the character of C-SVC, particularly with regard to the penalty term. We construct the primal problem and, thereafter, derive the dual problem. We introduce the notion of nonlinear classifiers and describe the so-called *kernel trick*. Additionally, we show how the primal problem can be derived from the dual problem. The paper is the second 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, the second in a series, we will describe the underlying mathematics of the soft-margin classifier C-SVC, the principal SVC in `scikit-learn`. We will make use of notation, terminology, and concepts from our previous paper [1], and the reader is advised to become familiar with that work before continuing here.

2 Soft-margin classifiers

Previously, we concerned ourselves only with hard-margin classifiers, in which the obtained margin does not contain any data points [1]. At most, the data points might lie on the edges of the margin, as in the previous examples, but not within the margin. A dataset that permits a hard margin to be found is said to be a *linearly separable* dataset, or simply *separable*.

Unfortunately, in real-world problems, datasets are usually not linearly separable. To find a practical separating margin, we need to allow the possibility that some data points might need to lie within the margin. Such a classifier is termed a **soft-margin classifier**. Soft classifiers are more generally applicable than hard classifiers, and it should come as no surprise that all of the classifiers in the `scikit-learn` SVC library are soft classifiers.

To develop an intuition for soft margin classifiers, consider Figure 1 on the next page. There are seven data points – three yellow, four red. The red points are all meant to be in the green area, and the yellow points are meant to be in the blue area. The central straight line is the decision surface, and the other two straight lines indicate the edges of the margin. The margin itself is the union of the light green and light blue areas.

All the red points are correctly classified since they are all in the green area. Two of them are located on the margin edge. We will refer to such points as *hard vectors*. One of them is located inside the margin (the light green area), and we will refer to such a point as a *soft vector*. Also, one red point is clearly located outside the margin.

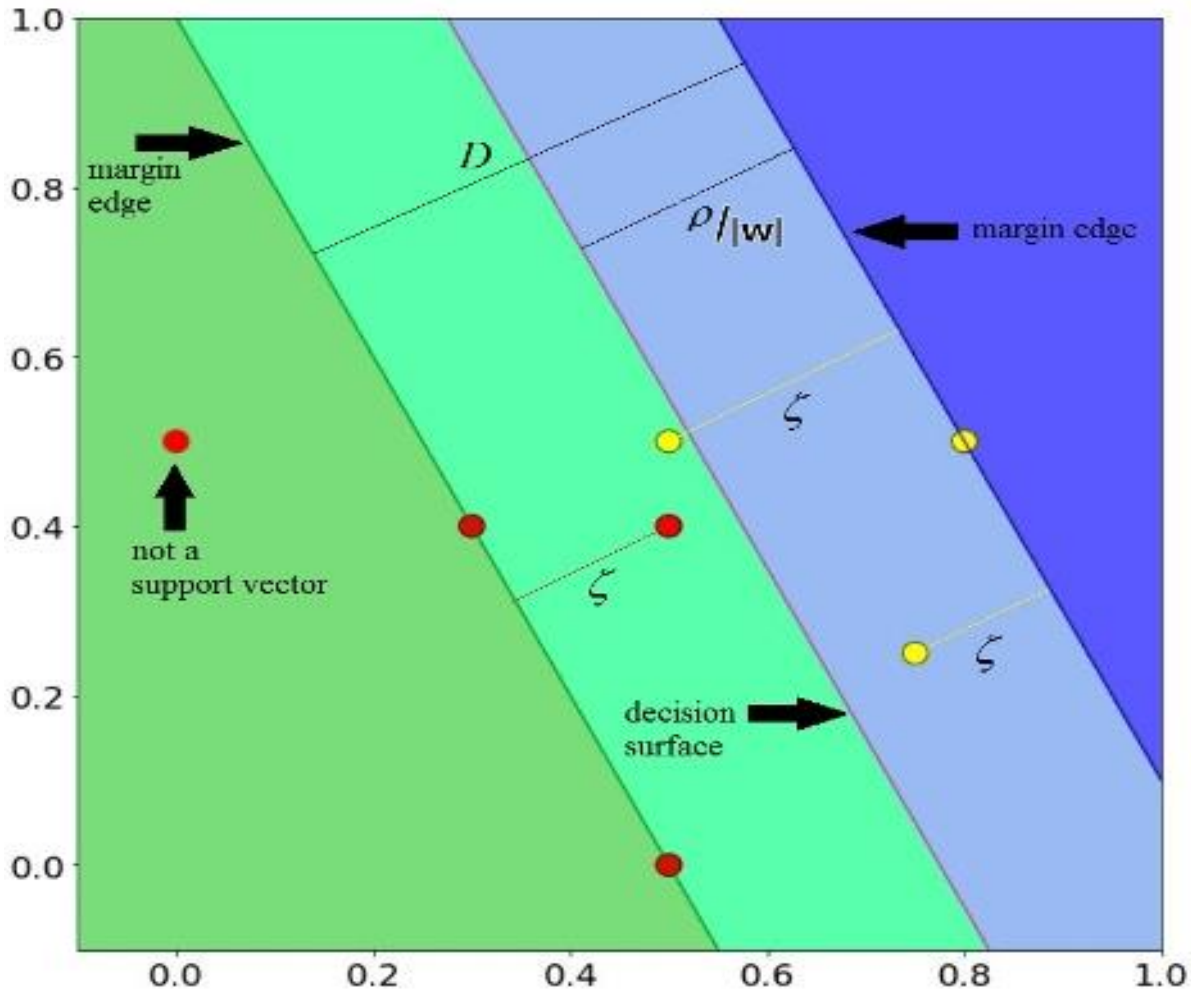

Figure 1: C = 10. Green and blue lines denote margin edges. Central pink line is the decision surface. Other relevant information is also shown.

One of the yellow points is a hard vector, and two are soft vectors. One of these soft vectors is incorrectly classified because it lies in the green area (i.e., on the wrong side of the decision surface).

In this calculation, we find that α_i for all the hard and soft vectors is nonzero. Hence, they are all support vectors. Only the red point at $(0,0.5)$ has $\alpha_i = 0$ and so is not a support vector. Each of the soft vectors has an associated parameter $\zeta_i > 0$. This parameter measures the distance of the soft vector from its respective margin edge. For the red vectors, this is the green line to the left of the decision surface; for the yellow vectors, it is the blue line to the right of the decision surface. Hard vectors, and all data points that are not support vectors, have $\zeta_i = 0$.

The parameters ζ_i are incorporated into the optimization problem by modifying the primal objective function F_p in the following way:

$$F_p(\mathbf{w},\zeta) = \frac{\mathbf{w}\cdot\mathbf{w}}{2} + C\sum_{i=1}^{N}\zeta_i.$$

The second term on the right is often called a *penalty* term. Both terms in this expression are nonnegative, and the process of minimizing this objective function essentially means that both terms must be kept simultaneously as small as possible. If the first term is made too small, then the margin will be very wide. This means that there will likely be many soft vectors, probably leading to the penalty term being large, particularly if the penalty parameter C is large. So, the `scikit-learn` optimization algorithm will try to avoid making the first term too small. On the other hand, if the penalty term is made very small there will be few, if any, soft vectors, implying a very narrow margin. But a narrow margin corresponds to a large value of $|\mathbf{w}|$, meaning that the first term could be too large. The optimization algorithm attempts to find the best balance between these extremes.

The penalty parameter C affects the width of the margin in an inverse manner. If C is large, the algorithm will attempt to keep the ζ_i small or zero. This means fewer soft vectors, implying that the margin is probably narrow. On the other hand, if C is small, larger values of ζ_i could be tolerated, suggesting the possibility of a wider margin.

In Figure 1, a value of $C = 10$ was used. In Figure 2, we use the same dataset, but with $C = 1000$. Clearly, a different decision surface has been found, and the margin is considerably narrower than before. There are three hard vectors and no soft vectors at all. The three hard vectors have nonzero α_i and so are support vectors. All the other data points have $\alpha_i = 0$.

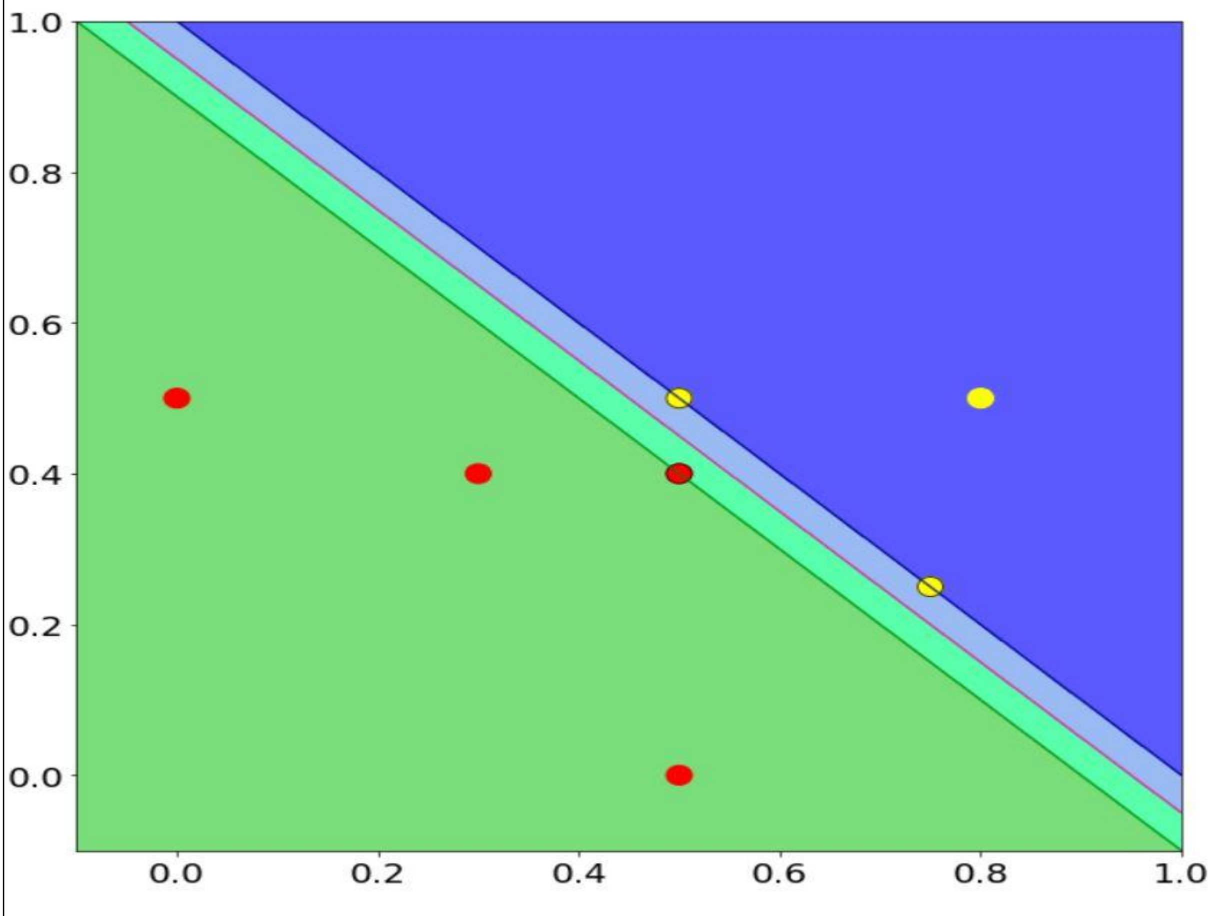

Figure 2: C = 1000. No soft vectors.

A classifier with the objective function F_p given above is often referred to as C-SVC. We will discuss the primal and dual problems for C-SVC in the next section.

3 C-SVC: Primal and dual problems

Using the expression for $F_p(\mathbf{w},\zeta)$ given previously, we may state the primal problem for C-SVC:

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

$$F_p(\mathbf{w},\zeta) = \frac{\mathbf{w}\cdot\mathbf{w}}{2} + C\sum_{i=1}^{N}\zeta_i$$

is minimized, and the constraints

$$y_i(\mathbf{w}\cdot\mathbf{x}_i + b) \geq 1 - \zeta_i,\ \zeta_i \geq 0$$

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

The $1-\zeta_i$ in the constraints reflects the softness of the classifier; we require that $y_i(\mathbf{w}\cdot\mathbf{x}_i + b)$ only be larger than a quantity that is possibly less than one, rather than one itself. These are less stringent constraints than for a hard classifier. Also note that there are now additional constraints on the problem, in the form $\zeta_i \geq 0$.

To derive the dual problem, we write the Lagrangian as

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

where the μ_i are KKT multipliers corresponding to the constraints $\zeta_i\geq 0$. The stationarity conditions give

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

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

$$\frac{\partial L}{\partial\zeta_i}=C-\alpha_i-\mu_i=0\;\Rightarrow\;\alpha_i+\mu_i=C\;\Rightarrow\;\alpha_i\leq C$$

where the last inequality is inferred from the fact that $\mu_i\geq 0$.

Some algebraic manipulation of the Lagrangian now gives

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

and, with $\sum_{i=1}^{N}\alpha_i y_i\mathbf{w}\cdot\mathbf{x}_i=\sum_{i=1}^{N}\alpha_i y_i\mathbf{x}_i\cdot\mathbf{w}=\mathbf{w}\cdot\mathbf{w}$, we find

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

so that

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

is the dual objective function.

The dual problem may now be stated:

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

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

is minimized, and the constraints

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

are satisfied.

The only difference between this formulation and that of the hard-margin classifier is the upper bound of C in the inequality constraints.

As with the hard-margin SVC, we have $\mathbf{w} = \sum_{i=1}^{N} y_i \alpha_i \mathbf{x}_i$, but the calculation of b is more complicated. To facilitate our analysis, we must make an important observation. The complementarity conditions for the soft classifier are

$$\alpha_i \left[y_i \left(\mathbf{w} \cdot \mathbf{x}_i + b \right) - 1 + \zeta_i \right] = 0$$
$$\mu_i \zeta_i = 0$$

and the stationarity condition $\frac{\partial L}{\partial \zeta_i} = 0$ gives

$$\alpha_i + \mu_i = C.$$

Consider data points with $0 < \alpha_i < C$. Using the above conditions, we reason as follows: since α_i is nonzero, we must have $y_i \left(\mathbf{w} \cdot \mathbf{x}_i + b \right) - 1 + \zeta_i = 0$. Since $\alpha_i < C$, we must have that $\mu_i \neq 0$, which implies that $\zeta_i = 0$. This, in turn, gives $y_i \left(\mathbf{w} \cdot \mathbf{x}_i + b \right) - 1 = 0$. This provides an expression for *b*, similar to the hard-margin case. For numerical stability, we take the average value over all support vectors with $0 < \alpha_i < C$

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

where Θ is the set of all support vectors with $0 < \alpha_i < C$, and N_Θ is the cardinality of Θ.

But what if Θ is empty? What if each data point has either $\alpha_i = 0$ or $\alpha_i = C$? First, we consider the case $\alpha_i = 0$. The primal constraints give $y_i \left(\mathbf{w} \cdot \mathbf{x}_i + b \right) - 1 + \zeta_i \geq 0$ and this does not violate the complementarity conditions, even if $\alpha_i = 0$. So, we have

$$
\begin{aligned}
& y_i(\mathbf{w}\cdot\mathbf{x}_i + b) - 1 + \zeta_i \geq 0 \\
\Rightarrow\ & y_i(\mathbf{w}\cdot\mathbf{x}_i + b) \geq 1 - \zeta_i \\
\Rightarrow\ & \begin{cases} \mathbf{w}\cdot\mathbf{x}_i + b \geq y_i - \zeta_i & (y_i = +1) \\ \mathbf{w}\cdot\mathbf{x}_i + b \leq \zeta_i + y_i & (y_i = -1) \end{cases} \\
\Rightarrow\ & \begin{cases} b \geq y_i - \mathbf{w}\cdot\mathbf{x}_i - \zeta_i & (y_i = +1) \\ b \leq y_i - \mathbf{w}\cdot\mathbf{x}_i + \zeta_i & (y_i = -1) \end{cases}
\end{aligned}
$$

When $\alpha_i = C$ we have, by virtue of the complementarity conditions,

$$
\begin{aligned}
& y_i(\mathbf{w}\cdot\mathbf{x}_i + b) - 1 + \zeta_i = 0 \\
\Rightarrow\ & \begin{cases} b = -\mathbf{w}\cdot\mathbf{x}_i + y_i - \zeta_i & (y_i = +1) \\ b = -\mathbf{w}\cdot\mathbf{x}_i + y_i + \zeta_i & (y_i = -1) \end{cases} \\
\Rightarrow\ & \begin{cases} -b = -y_i + \mathbf{w}\cdot\mathbf{x}_i + \zeta_i & (y_i = +1) \\ \ \ b = y_i - \mathbf{w}\cdot\mathbf{x}_i + \zeta_i & (y_i = -1) \end{cases} \\
\Rightarrow\ & \left.\begin{cases} -b \geq -y_i + \mathbf{w}\cdot\mathbf{x}_i & (y_i = +1) \\ \ \ b \geq y_i - \mathbf{w}\cdot\mathbf{x}_i & (y_i = -1) \end{cases}\right\} \text{since } \zeta_i \geq 0 \\
\Rightarrow\ & \begin{cases} b \leq y_i - \mathbf{w}\cdot\mathbf{x}_i & (y_i = +1) \\ b \geq y_i - \mathbf{w}\cdot\mathbf{x}_i & (y_i = -1) \end{cases}
\end{aligned}
$$

The inequalities highlighted in red and blue are properties of b – whatever the value of b, it must satisfy those inequalities.

Now, define two sets

$$
\begin{aligned}
A_L &= \{y_i - \mathbf{w}\cdot\mathbf{x}_i \mid y_i = +1 \text{ and } \alpha_i = 0\} \cup \{y_i - \mathbf{w}\cdot\mathbf{x}_i \mid y_i = -1 \text{ and } \alpha_i = C\} \\
A_U &= \{y_i - \mathbf{w}\cdot\mathbf{x}_i \mid y_i = -1 \text{ and } \alpha_i = 0\} \cup \{y_i - \mathbf{w}\cdot\mathbf{x}_i \mid y_i = +1 \text{ and } \alpha_i = C\}
\end{aligned}
$$

and then choose

$$
b = \frac{\max A_L + \min A_U}{2}.
$$

This choice of b ensures that

$$\max A_L \leq b \leq \min A_U$$

and, since $\zeta_i \geq 0$, this means that b satisfies the red and blue inequalities highlighted above.

This is the prescription used in the `scikit-learn` library, although we acknowledge that, if $\max A_L \neq \min A_U$, then there are actually infinitely many possible choices of b in the interval $[\max A_L, \min A_U]$.

Throughout this discussion we have assumed that the parameter C is single-valued. This is the default assumption in the `scikit-learn` algorithms, which require that C be user-specified. However, a more specialized approach to C-SVC is possible. We can replace C with C_i so that F_p becomes

$$F_p(\mathbf{w}) = \frac{\mathbf{w} \cdot \mathbf{w}}{2} + \sum_{i=1}^{N} C_i \zeta_i .$$

In other words, a penalty parameter C_i is specified for each data point (this is known as *sample weighting*). Very often, this is done in such a way that elements of S_- each have the same penalty parameter, and elements of S_+ each have the same penalty parameter, but such that these two penalty parameters themselves have different values. This results in each class having a different penalty parameter and is known as *class weighting*.

Whatever approach is taken, the net result is that the stationarity condition becomes

$$\frac{\partial L}{\partial \zeta_i} = C_i - \alpha_i - \mu_i = 0 \;\Rightarrow\; \alpha_i + \mu_i = C_i \;\Rightarrow\; \alpha_i \le C_i$$

so that each α_i now has its own upper bound. This has ramifications for the decision surface, but such a discussion is outside the scope of this paper.

4 Nonlinear SVCs

Up to now, we have considered only linearly separable datasets. Strictly speaking, a linearly separable dataset is one for which a hard-margin solution can be found, by solving either the primal or dual problems that we have encountered thus far. If a hard-margin solution is not possible, but an acceptable soft-margin solution can be found, then we would probably still be willing to regard the dataset as linearly separable, in a pragmatic sense.

But consider the following case: assume the unit square is populated with N data points. Draw a circle of radius 0.2 in the centre of the square. Define S_- to be the set of all points inside the circle, and S_+ to be all the other points. Clearly, the two sets of points are separated by a circle, not a straight line and, since the points in S_- are surrounded by the points in S_+, any soft margin solution would likely be a very poor solution indeed. In such a case, many of the points from both sets would be misclassified, and the resulting classifier would be of very low quality.

The approach to solving this problem is to map the input space (the unit square, in this case) to a **feature space**, such that the dataset is separable in the feature space. Considering our example above, we see that the points in S_- satisfy

$$\left(x_1-0.5\right)^2+\left(x_2-0.5\right)^2\leq 0.2^2=0.04.$$

Now define

$$\begin{aligned}
\varphi_1\left(\mathbf{x}\right)&=\varphi_1\left(x_1,x_2\right)=\left(x_1-0.5\right)^2\\
\varphi_2\left(\mathbf{x}\right)&=\varphi_2\left(x_1,x_2\right)=\left(x_2-0.5\right)^2\\
\boldsymbol{\varphi}\left(\mathbf{x}\right)&=\left(\varphi_1\left(\mathbf{x}\right),\varphi_2\left(\mathbf{x}\right)\right).
\end{aligned}$$

These maps allow the separating curve (the circle) to be written as

$$\varphi_1+\varphi_2=0.04\ \Rightarrow\ \varphi_2=-\varphi_1+0.04$$

which, of course, is a straight line in the $\left(\varphi_1,\varphi_2\right)$ space. The map $\boldsymbol{\varphi}$ transforms a vector $\mathbf{x}=\left(x_1,x_2\right)$ in the input space to a vector $\boldsymbol{\varphi}\left(\mathbf{x}\right)=\left(\varphi_1\left(\mathbf{x}\right),\varphi_2\left(\mathbf{x}\right)\right)$ in the feature space.

The original data still resides in the input space, where it is not linearly separable. The transformed data in the feature space, however, is separable, and this is what we seek to exploit.

To now construct an SVC in this scenario, we simply solve the optimization problem (primal or dual) in the feature space, using $\boldsymbol{\varphi}\left(\mathbf{x}_i\right)\cdot\boldsymbol{\varphi}\left(\mathbf{x}_j\right)$ in place of $\mathbf{x}_i\cdot\mathbf{x}_j$.

The primal problem for *C*-SVC can now be stated as follows:

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

$$F_p(\mathbf{w}) = \frac{\mathbf{w}\cdot\mathbf{w}}{2} + C\sum_{i=1}^{N}\zeta_i$$

is minimized, and the constraints

$$y_i\left(\mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i)+b\right) \geq 1-\zeta_i,\ \zeta_i \geq 0$$

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

The function $K(\mathbf{x}_i, \mathbf{x}_j) = \boldsymbol{\varphi}(\mathbf{x}_i)\cdot\boldsymbol{\varphi}(\mathbf{x}_j)$, which will appear in the dual problem (see p17), is known as the *inner-product kernel*. If

$$\boldsymbol{\varphi}(\mathbf{x}_i) = \left(\varphi_1(\mathbf{x}_i), \varphi_2(\mathbf{x}_i), \ldots, \varphi_{\Pi}(\mathbf{x}_i)\right)$$

then

$$\begin{aligned} K(\mathbf{x}_i, \mathbf{x}_j) &= \boldsymbol{\varphi}(\mathbf{x}_i)\cdot\boldsymbol{\varphi}(\mathbf{x}_j) \\ &= \left(\varphi_1(\mathbf{x}_i), \ldots, \varphi_{\Pi}(\mathbf{x}_i)\right)\cdot\left(\varphi_1(\mathbf{x}_j), \ldots, \varphi_{\Pi}(\mathbf{x}_j)\right) \\ &= \sum_{k=1}^{\Pi}\varphi_k(\mathbf{x}_i)\ \varphi_k(\mathbf{x}_j) = \sum_{k=1}^{\Pi}\varphi_k(\mathbf{x}_j)\ \varphi_k(\mathbf{x}_i) \\ &= K(\mathbf{x}_j, \mathbf{x}_i) \end{aligned}$$

which shows that the kernel is *symmetric* in its arguments. We note here that the dimensionality Π of the feature space does not need to be the same as the dimensionality M of the input space.

The vector $\mathbf{x}$ denotes a generic vector in the input space; hence, the vector $\boldsymbol{\varphi}(\mathbf{x})$ is the corresponding generic vector in the feature space. When we solve the dual problem stated above, we have the expansion

$$\mathbf{w} = \sum_{i=1}^{N} y_i \alpha_i \boldsymbol{\varphi}(\mathbf{x}_i)$$

so that

$$\mathbf{w} \cdot \boldsymbol{\varphi}(\mathbf{x}) = \sum_{i=1}^{N} y_i \alpha_i \boldsymbol{\varphi}(\mathbf{x}_i) \cdot \boldsymbol{\varphi}(\mathbf{x}) = \sum_{i=1}^{N} y_i \alpha_i K(\mathbf{x}_i, \mathbf{x}).$$

The decision surface in the feature space is thus given by

$$\mathbf{w} \cdot \boldsymbol{\varphi}(\mathbf{x}) + b = 0$$
$$\Rightarrow \sum_{i=1}^{N} y_i \alpha_i K(\mathbf{x}_i, \mathbf{x}) + b = 0$$

where $\mathbf{w}$ in this context is a Π**–dimensional vector in the feature space.**

We also find

$$\mathbf{w}^2 = \mathbf{w} \cdot \mathbf{w} = \left(\sum_{i=1}^{N} y_i \alpha_i \boldsymbol{\varphi}(\mathbf{x}_i) \right) . \left(\sum_{j=1}^{N} y_j \alpha_j \boldsymbol{\varphi}(\mathbf{x}_j) \right)$$
$$= \sum_{i=1}^{N} \sum_{j=1}^{N} y_i \alpha_i y_j \alpha_j \boldsymbol{\varphi}(\mathbf{x}_i) \cdot \boldsymbol{\varphi}(\mathbf{x}_j)$$
$$= \sum_{i=1}^{N} \sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j)$$

and

$$\left|\mathbf{w}\right| = \sqrt{\sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j K\left(\mathbf{x}_i, \mathbf{x}_j\right)}$$

and, if $\mathbf{z}$ is a test point in the input space, then

$$\overline{\Delta}\left(\boldsymbol{\varphi}\left(\mathbf{z}\right) \middle| \mathbf{w}, b\right) = \frac{\sum_{i=1}^{N} y_i \alpha_i K\left(\mathbf{x}_i, \mathbf{z}\right) + b}{\left|\mathbf{w}\right|} = \frac{\sum_{i=1}^{N} y_i \alpha_i K\left(\mathbf{x}_i, \mathbf{z}\right) + b}{\sqrt{\sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j K\left(\mathbf{x}_i, \mathbf{x}_j\right)}}$$

is the signed distance between $\boldsymbol{\varphi}\left(\mathbf{z}\right)$ and the decision surface in the feature space. We also modify the expressions for the intercept *b*, as in

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

where Θ is the set of all support vectors with $0 < \alpha_i < C$, and N_Θ is the cardinality of Θ, or we define the sets

$$A_L = \left\{ y_i - \mathbf{w}\cdot\boldsymbol{\varphi}\left(\mathbf{x}_i\right) \middle| y_i = +1 \text{ and } \alpha_i = 0 \right\} \cup \left\{ y_i - \mathbf{w}\cdot\boldsymbol{\varphi}\left(\mathbf{x}_i\right) \middle| y_i = -1 \text{ and } \alpha_i = C \right\}$$
$$A_U = \left\{ y_i - \mathbf{w}\cdot\boldsymbol{\varphi}\left(\mathbf{x}_i\right) \middle| y_i = -1 \text{ and } \alpha_i = 0 \right\} \cup \left\{ y_i - \mathbf{w}\cdot\boldsymbol{\varphi}\left(\mathbf{x}_i\right) \middle| y_i = +1 \text{ and } \alpha_i = C \right\}$$

and then choose

$$b = \frac{\max A_L + \min A_U}{2}.$$

We note again that $\mathbf{w}\cdot\boldsymbol{\varphi}\left(\mathbf{x}_i\right) = \sum_{j=1}^{N} y_j \alpha_j \boldsymbol{\varphi}\left(\mathbf{x}_j\right)\cdot\boldsymbol{\varphi}\left(\mathbf{x}_i\right) = \sum_{j=1}^{N} y_j \alpha_j K\left(\mathbf{x}_j, \mathbf{x}_i\right)$.

The most significant aspect of this nonlinear transformation is revealed in the restatement of the dual problem

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

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

is minimized, and the constraints

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

are satisfied.

We see that the kernel $K(\mathbf{x}_i, \mathbf{x}_j)$ replaces the scalar product $\boldsymbol{\varphi}(\mathbf{x}_i)\cdot\boldsymbol{\varphi}(\mathbf{x}_j)$, so that the map $\boldsymbol{\varphi}$ does not need to be known explicitly. Also, we only need the kernel for computing $\mathbf{w}\cdot\boldsymbol{\varphi}$ and *b*, as well. This capability of a nonlinear SVC to replace knowledge of the map $\boldsymbol{\varphi}$ simply with an appropriate scalar function is known as the **'kernel trick'**.

In order for a scalar function to serve as a kernel, it is necessary and sufficient that the so-called *Gram* matrix $\mathbf{K}$, whose elements are given by $K(\mathbf{x}_i, \mathbf{x}_j)$, should be *positive semidefinite* for all possible combinations of $\mathbf{x}_i$ and $\mathbf{x}_j$ drawn from the dataset $S_- \cup S_+$.

A positive semidefinite matrix is a *Hermitian* matrix, of which all eigenvalues are nonnegative. A Hermitian matrix is a square matrix that is equal to its own conjugate transpose. We know the kernel is symmetric in its arguments, i.e., $K\left(\mathbf{x}_i, \mathbf{x}_j\right) = K\left(\mathbf{x}_j, \mathbf{x}_i\right)$. If the kernel is also real-valued, then $\mathbf{K}$ is necessarily Hermitian.

Examples of nonlinear kernels include the popular *radial basis function* (RBF) kernel

$$K\left(\mathbf{x}_i, \mathbf{x}_j\right) = \exp\left(-\gamma \left\| \mathbf{x}_i - \mathbf{x}_j \right\|^2\right),$$

the *polynomial* kernel

$$K\left(\mathbf{x}_i, \mathbf{x}_j\right) = \left(\gamma \left\langle \mathbf{x}_i, \mathbf{x}_j \right\rangle + r\right)^d,$$

and the *sigmoid* kernel

$$K\left(\mathbf{x}_i, \mathbf{x}_j\right) = \tanh\left(\gamma \left\langle \mathbf{x}_i, \mathbf{x}_j \right\rangle + r\right),$$

where $\langle \cdot \rangle$ is an inner product, and $\|\cdot\|$ is a norm (usually taken as the scalar product and Euclidean distance, respectively). The parameters γ, r and d, known as hyperparameters, are user-specified.

Lastly, we note that a linear SVC is simply a nonlinear SVC with

$$\begin{aligned} \boldsymbol{\varphi}\left(\mathbf{x}_i\right) &= \mathbf{x}_i \\ K\left(\mathbf{x}_i, \mathbf{x}_j\right) &= \boldsymbol{\varphi}\left(\mathbf{x}_i\right) \cdot \boldsymbol{\varphi}\left(\mathbf{x}_j\right) = \mathbf{x}_i \cdot \mathbf{x}_j. \end{aligned}$$

Unsurprisingly, this kernel is known as the *linear* kernel.

5 Deriving the primal from the dual

We derive the primal problem from the dual problem for C-SVC, using the nonlinear formulation.

C-SVC

In the C-SVC dual problem, the only additional aspect is the upper bound

$$\alpha_i \leq C.$$

This is incorporated into the Lagrangian by means of the term

$$-\sum_{i=1}^{N} \zeta_i (C - \alpha_i) = -C \sum_{i=1}^{N} \zeta_i + \sum_{i=1}^{N} \zeta_i \alpha_i$$

where the $\zeta_i \geq 0$ are KKT multipliers. The derivative of this term with respect to α_i gives the term ζ_i, and so we find

$$y_i \sum_{j=1}^{N} \alpha_j y_j \boldsymbol{\varphi}(\mathbf{x}_j) \cdot \boldsymbol{\varphi}(\mathbf{x}_i) = 1 - b y_i - \zeta_i + \mu_i$$
$$\Rightarrow y_i \left(\mathbf{w} \cdot \boldsymbol{\varphi}(\mathbf{x}_i) + b \right) \geq 1 - \zeta_i$$

which are the familiar primal conditions for C-SVC.

Including the additional term in the Lagrangian gives the following expression

$$L(\alpha, b, \mu, \zeta) = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j) - \sum_{i=1}^{N} \alpha_i + b \sum_{i=1}^{N} y_i \alpha_i - \sum_{i=1}^{N} \mu_i \alpha_i$$
$$- C \sum_{i=1}^{N} \zeta_i + \sum_{i=1}^{N} \zeta_i \alpha_i$$

$$= \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y_i y_j K\left(\mathbf{x}_i,\mathbf{x}_j\right) - C\sum_{i=1}^{N}\zeta_i$$

$$-\sum_{i=1}^{N}\alpha_i\left(1 - by_i - \zeta_i + \mu_i\right)$$

$$= \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y_i y_j K\left(\mathbf{x}_i,\mathbf{x}_j\right) - C\sum_{i=1}^{N}\zeta_i$$

$$-\sum_{i=1}^{N}\alpha_i y_i\sum_{j=1}^{N}\alpha_j y_j K\left(\mathbf{x}_j,\mathbf{x}_i\right)$$

$$= -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y_i y_j K\left(\mathbf{x}_i,\mathbf{x}_j\right) - C\sum_{i=1}^{N}\zeta_i.$$

This leads to

$$F_p\left(\mathbf{w},\zeta\right) = -L\left(\alpha,\zeta\right) = \frac{\mathbf{w}\cdot\mathbf{w}}{2} + C\sum_{i=1}^{N}\zeta_i$$

as expected for *C*-SVC. To cater for weighted *C*-SVC we simply replace the term $C\sum_{i=1}^{N}\zeta_i$ with $\sum_{i=1}^{N}C_i\zeta_i$ throughout, to get

$$F_p\left(\mathbf{w},\zeta\right) = -L\left(\alpha,\zeta\right) = \frac{\mathbf{w}\cdot\mathbf{w}}{2} + \sum_{i=1}^{N}C_i\zeta_i.$$

6 Concluding comments

We have described the soft-margin classifier *C*-SVC in detail and provided insight into the nature of nonlinear SVCs. In the next paper in this series, we will discuss the soft-margin classifier known as *ν*-SVC and implemented in **`scikit-learn`** as `svm.NuSVC`.

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We reproduce the bibliography from [1], with a few additional items.

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