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

J.S.C. Prentice

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

August 21, 2023

Abstract

We present mathematical detail pertaining to the theory of the soft-margin support vector classifier ν-SVC, as used in `scikit-learn`. We construct the primal problem, from which we derive the dual problem. We also show how the primal problem can be derived from the dual problem. We analyse the effect of the parameter ν, and we discuss the relationship between ν-SVC and C-SVC. We include an interesting numerical example. The paper is the third 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 third in a series, we will describe the underlying mathematics of the soft-margin classifier ν-SVC. We will make use of notation, terminology, and concepts from our previous papers [1, 2], and our readers are advised to familiarise themselves with those works before continuing here.

2 ν-SVC: Primal and dual problems

In our earlier paper [1], we presented the primal problem in the following form:

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 $i = 1, 2, \ldots, N$.

Thereafter, we scaled the problem by dividing by ρ, so that ρ effectively became an arbitrary parameter.

However, it is possible to define the problem so that ρ is a parameter to be determined. In such a case, since $D = 2\rho / |\mathbf{w}|$, it is clear that not only do we seek to minimize $|\mathbf{w}|$, but we also seek to maximize ρ. such a classifier is known as ν-SVC (pronounced 'new'-SVC) and has certain desirable properties, as we shall see.

The most general form of the ν-SVC primal problem is

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

$$F_p(\mathbf{w}, \rho, \zeta) = \frac{\mathbf{w}\cdot\mathbf{w}}{2} + C_\nu \sum_{i=1}^{N} \zeta_i - \nu\rho \qquad (C_\nu, \nu > 0)$$

is minimized, and the constraints

$$\begin{aligned} & y_i\left(\mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i) + b\right) \geq \rho - \zeta_i \\ & \zeta_i \geq 0,\ \rho \geq 0 \end{aligned}$$

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

Here, we have retained our familiar notation $(\mathbf{w},\ b,\ \zeta)$ and we have introduced two new strictly positive parameters C_ν and ν. These parameters indicate the weight of their respective terms, relative to the first term. The negative sign in the ρ term is necessary because, although we seek to maximize ρ, we also seek to simultaneously **minimize** F_p. For the sake of generality, we have also used notation consistent with a nonlinear problem – $\boldsymbol{\varphi}(\mathbf{x}_i)$ instead of $\mathbf{x}_i$ – and we are clearly describing a soft margin classifier by incorporating the ζ term.

In principle, the parameter C_ν can be arbitrary, but we will see shortly that a particular choice is meaningful. Also, we will find that ν is actually bounded above. Firstly, though, we will derive the dual problem for ν-SVC.

We write the Lagrangian as

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

where α, μ and η are KKT multipliers. The stationarity conditions give

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

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

$$\frac{\partial L}{\partial \rho} = -\nu - \eta + \sum_{i=1}^{N} \alpha_i = 0 \Rightarrow \sum_{i=1}^{N} \alpha_i = \nu + \eta$$

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

Substituting these into the expression for the Lagrangian gives

$$L = \frac{\mathbf{w}\cdot\mathbf{w}}{2} - \sum_{i=1}^{N} \alpha_i y_i \mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i) - b\sum_{i=1}^{N} \alpha_i y_i + C_v \sum_{i=1}^{N} \zeta_i$$
$$- \sum_{i=1}^{N} \alpha_i \zeta_i - \sum_{i=1}^{N} \mu_i \zeta_i - \nu\rho - \eta\rho + \sum_{i=1}^{N} \alpha_i \rho$$
$$= \frac{\mathbf{w}\cdot\mathbf{w}}{2} - \sum_{i=1}^{N} \alpha_i y_i \mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i) - b\sum_{i=1}^{N} \alpha_i y_i + \sum_{i=1}^{N} (C_v - \alpha_i - \mu_i)\zeta_i$$
$$+ \rho\left(\sum_{i=1}^{N} \alpha_i - \nu - \eta \right)$$
$$= \frac{\mathbf{w}\cdot\mathbf{w}}{2} - \mathbf{w}\cdot\mathbf{w} - 0 + 0 + 0 = -\frac{\mathbf{w}\cdot\mathbf{w}}{2}$$

where we have used $\sum_{i=1}^{N} \alpha_i y_i \mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i) = \sum_{i=1}^{N} \alpha_i y_i \boldsymbol{\varphi}(\mathbf{x}_i)\cdot\mathbf{w} = \mathbf{w}\cdot\mathbf{w}$.

Hence,

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

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

and so

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

Two conditions have arisen from the stationarity conditions: $\alpha_i \le C_v$ and $\sum_{i=1}^{N}\alpha_i = v + \eta$. If $\rho > 0$, as might be expected in a soft classifier, $\eta = 0$ (by the complementarity condition $\eta\rho = 0$), and so we have $\sum_{i=1}^{N}\alpha_i = v$. On the other hand, imposing $\sum_{i=1}^{N}\alpha_i = v$ *a priori* does not preclude $\rho = 0$, because $\eta\rho = 0$ is obviously satisfied if both η and ρ are zero. It seems reasonable, then, to impose $\sum_{i=1}^{N}\alpha_i = v$ as a condition on the dual problem. In addition, if we choose $C_v = 1/N$, we then have the condition $0 \le \alpha_i \le 1/N$.

We now scale α_i according to

$$\tilde{\alpha}_i = \alpha_i N$$

and we have

$$0 \le \tilde{\alpha}_i \le 1$$

$$\sum_{i=1}^{N}\tilde{\alpha}_i = vN.$$

We can now redefine F_d in terms of $\tilde{\alpha}_i$ as

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

and similarly for $\mathbf{w}$

$$\begin{aligned} \mathbf{w} &= \sum_{i=1}^{N} y_i \alpha_i \boldsymbol{\varphi}(\mathbf{x}_i) \\ &= \frac{1}{N} \sum_{i=1}^{N} y_i \tilde{\alpha}_i \boldsymbol{\varphi}(\mathbf{x}_i). \end{aligned}$$

Of course, minimizing $N^2 F_d(\tilde{\alpha})$ is equivalent to minimizing $F_d(\tilde{\alpha})$ itself, so we may drop the N^2 from the coefficient of $F_d(\tilde{\alpha})$, and state the dual problem for ν-SVC as follows:

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

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

is minimized, and the constraints

$$\begin{aligned} &0 \le \tilde{\alpha}_i \le 1 \quad \text{for } i = 1, 2, \ldots, N \\ &\sum_{i=1}^{N} \tilde{\alpha}_i y_i = 0 \\ &\sum_{i=1}^{N} \tilde{\alpha}_i = \nu N \end{aligned}$$

are satisfied.

The scaling $\tilde{\alpha}_i = \alpha_i N$ is done primarily for the sake of numerical stability. If N is very large, then $1/N$ is very small, likely leading to very small values of α_i. This, in turn, gives extremely small values for the product $\alpha_i \alpha_j$ in F_d, and the algorithm could become contaminated by roundoff error. The scaling ensures that the $\tilde{\alpha}_i$ are likely to have larger values and the product $\alpha_i \alpha_j$ is likely to be larger than machine precision. However, this scaling also exposes the significance of the choice $C_v = 1/N$. After the scaling, we have the conditions

$$0 \le \tilde{\alpha}_i \le 1 \qquad \sum_{i=1}^{N} \tilde{\alpha}_i = vN.$$

Since each $\tilde{\alpha}_i$ is bounded by one, the sum $\sum_{i=1}^{N} \tilde{\alpha}_i$ is bounded by N_S, where N_S denotes the number of support vectors. Hence,

$$\sum_{i=1}^{N} \tilde{\alpha}_i \le N_S \;\Rightarrow\; vN \le N_S \;\Rightarrow\; v \le \frac{N_S}{N} \le 1$$

so that v is a **lower bound** on the fraction of data points that are support vectors. Let N_ζ denote the number of data points with $\zeta_i \ne 0$ $(\Rightarrow \tilde{\alpha}_i = 1)$ and let N_0 denote the number of data points with $\zeta_i = 0$ $(\Rightarrow \tilde{\alpha}_i < 1)$. Then we find

$$\sum_{i=1}^{N} \tilde{\alpha}_i = N_\zeta + N_0 \bar{\tilde{\alpha}}$$

where $\bar{\tilde{\alpha}}$ is the mean value of $\tilde{\alpha}_i$ for those data points with $\zeta_i = 0$. This gives

$$\nu N = N_\zeta + N_0 \bar{\tilde{\alpha}} \Rightarrow \nu = \frac{N_\zeta}{N} + \frac{N_0 \bar{\tilde{\alpha}}}{N} \Rightarrow \nu \geq \frac{N_\zeta}{N} \geq 0$$

and we see that ν is an **upper bound** on the fraction of data points with $\zeta_i \neq 0$ (i.e., soft vectors). This analysis also shows that $0 < \nu \leq 1$ (we do not consider $\nu = 0$, as discussed in the note at the end of this section (p12)). In fact, it has been shown that ν should be chosen such that

$$0 < \nu \leq \frac{2 \min\{N_-, N_+\}}{N}$$

where N_- and N_+ are the cardinalities of S_- and S_+, respectively, or else the problem does not have a feasible solution [12, 14]. Note that

$$\frac{\min\{N_-, N_+\}}{N} \leq \frac{1}{2}$$

means that we necessarily have $\nu \not> 1$.

The implication of this analysis is that ν can be chosen with a bound on the number of support vectors in mind, or a bound on the number of soft vectors in mind, thus giving some control to the user in these regards. Of course, all of this is made possible through the particular choice $C_\nu = 1/N$.

The calculation of b and ρ is similar to that for C-SVC. First, let us assume that we have at least one hard support vector $(0 < \alpha_i < C_\nu)$. For hard vectors, $\zeta_i = 0$ and the primal conditions give

$$\mathbf{w} \cdot \boldsymbol{\varphi}(\mathbf{x}_i) + b - y_i \rho = 0.$$

Hence,

$$b+\rho=-\mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i) \qquad y_i=-1$$
$$b-\rho=-\mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i) \qquad y_i=+1$$

We take average values over all hard support vectors, as in

$$b+\rho=-\frac{1}{N_-^H}\sum_{\mathbf{x}_i\in H_-}\mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i)$$
$$b-\rho=-\frac{1}{N_+^H}\sum_{\mathbf{x}_i\in H_+}\mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i)$$

where H_- is the set of hard support vectors in S_-, H_+ is the set of hard support vectors in S_+, N_-^H is the cardinality of H_- and N_+^H is the cardinality of H_+. These can be solved to give

$$b=-\frac{1}{2}\left(\frac{1}{N_-^H}\sum_{\mathbf{x}_i\in H_-}\mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i)+\frac{1}{N_+^H}\sum_{\mathbf{x}_i\in H_+}\mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i)\right)$$
$$\rho=-\frac{1}{2}\left(\frac{1}{N_-^H}\sum_{\mathbf{x}_i\in H_-}\mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i)-\frac{1}{N_+^H}\sum_{\mathbf{x}_i\in H_+}\mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i)\right).$$

If there are no hard support vectors, we define the sets

$$B_L^+=\left\{-\mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i)\middle| y_i=+1 \text{ and } \alpha_i=0\right\}$$
$$B_U^+=\left\{-\mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i)\middle| y_i=+1 \text{ and } \alpha_i=C_v\right\}$$
$$B_L^-=\left\{-\mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i)\middle| y_i=-1 \text{ and } \alpha_i=C_v\right\}$$
$$B_U^-=\left\{-\mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i)\middle| y_i=-1 \text{ and } \alpha_i=0\right\}$$

and use

$$b-\rho=\frac{\max B_L^+ + \min B_U^+}{2}$$
$$b+\rho=\frac{\max B_L^- + \min B_U^-}{2}$$

to find

$$b=\frac{\max B_L^+ + \min B_U^+ + \max B_L^- + \min B_U^-}{4}$$

$$\rho=\frac{\max B_L^- + \min B_U^- - \max B_L^+ - \min B_U^+}{4}.$$

We note that

$$\mathbf{w}=\sum_{j=1}^{N} y_j\alpha_j\boldsymbol{\varphi}(\mathbf{x}_j) \Rightarrow \mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{x}_i)=\sum_{j=1}^{N} y_j\alpha_j\boldsymbol{\varphi}(\mathbf{x}_j)\cdot\boldsymbol{\varphi}(\mathbf{x}_i)$$
$$=\sum_{j=1}^{N} y_j\alpha_j K(\mathbf{x}_j,\mathbf{x}_i).$$

This analysis holds for the *unscaled* solution α_i. For the scaled solution $\tilde{\alpha}_i$, simply replace α_i with $\tilde{\alpha}_i$, C_ν with 1, and $\mathbf{w}=\sum_{i=1}^{N} y_i\alpha_i\boldsymbol{\varphi}(\mathbf{x}_i)$ with $\mathbf{w}=\frac{1}{N}\sum_{i=1}^{N} y_i\tilde{\alpha}_i\boldsymbol{\varphi}(\mathbf{x}_i)$.

In our last study in this section, we will examine the relationship between ν-SVC and C-SVC. Assume we solve the ν-SVC dual problem and obtain a value of $\rho>0$. We can manipulate F_p as follows:

$$F_p(\mathbf{w},\rho,\zeta)=\rho^2\left(\frac{\frac{\mathbf{w}}{\rho}\cdot\frac{\mathbf{w}}{\rho}}{2}+\frac{1}{N\rho}\sum_{i=1}^{N}\frac{\zeta_i}{\rho}-\frac{\nu\rho}{\rho^2}\right)$$
$$\equiv\rho^2\left(\frac{\mathbf{w}'\cdot\mathbf{w}'}{2}+\frac{1}{N\rho}\sum_{i=1}^{N}\zeta_i'-\nu'\right)$$

In other words, we scale the primal objective function by dividing by ρ^2. We can also scale the primal conditions, by dividing by ρ, to get

$$y_i\left(\frac{\mathbf{w}}{\rho}\cdot\boldsymbol{\varphi}(\mathbf{x}_i)+\frac{b}{\rho}\right)\geq\frac{\rho}{\rho}-\frac{\zeta_i}{\rho}\Rightarrow y_i\left(\mathbf{w}'\cdot\boldsymbol{\varphi}(\mathbf{x}_i)+b'\right)\geq 1-\zeta_i'.$$

Since ν is user-defined and ρ is known, $\nu'=\nu/\rho$ is a known constant. Hence, minimizing $\rho^2\left(\frac{\mathbf{w}'\cdot\mathbf{w}'}{2}+\frac{1}{N\rho}\sum_{i=1}^{N}\zeta_i'-\nu'\right)$ is equivalent to minimizing $\left(\frac{\mathbf{w}'\cdot\mathbf{w}'}{2}+\frac{1}{N\rho}\sum_{i=1}^{N}\zeta_i'\right)$. But minimizing

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

subject to

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

is nothing more than a C-SVC problem, in which the unknown quantities are $\mathbf{w}'$, b' and ζ', and where the relevant value of C has been highlighted. Now, we have

$$\begin{aligned}\mathbf{w}'&=\frac{\mathbf{w}}{\rho}=\frac{1}{\rho}\sum_{j=1}^{N}y_j\alpha_j\boldsymbol{\varphi}(\mathbf{x}_j)\\&=\sum_{j=1}^{N}y_j\frac{\alpha_j}{\rho}\boldsymbol{\varphi}(\mathbf{x}_j)=\sum_{j=1}^{N}y_j\frac{N\alpha_j}{N\rho}\boldsymbol{\varphi}(\mathbf{x}_j)\\&=\sum_{j=1}^{N}y_j\frac{\tilde{\alpha}_i}{N\rho}\boldsymbol{\varphi}(\mathbf{x}_j).\end{aligned}$$

But $\tilde{\alpha}_i$ is the solution of the ν-SVC dual problem which yielded the solution ρ. Hence, we see that

$$\frac{\tilde{\alpha}_i}{N\rho}=\frac{N\alpha_i}{N\rho}=\frac{\alpha_i}{\rho}$$

is the solution to the C-SVC problem, when $C = 1/N\rho$. This means that any ν-SVC solution, suitably scaled, is a C-SVC solution (when C is chosen appropriately). The implication is that the ν-SVC solution set is a subset of the C-SVC solution set.

In truth, this relationship between ν-SVC and C-SVC is probably more of academic interest than practical interest. Nevertheless, it is important for our purposes to understand this relationship, because the **scikit-learn** algorithm **NuSVC** outputs the ν-SVC solution in scaled form, and if we wish to recover the 'true' ν-SVC solution, we need to be able to determine ρ (which is not a direct output of **NuSVC**) in order to reverse the scaling. We have

$$\sum_{i=1}^{N}\left(\frac{\tilde{\alpha}_i}{N\rho}\right) = \frac{1}{N\rho}\sum_{i=1}^{N}\tilde{\alpha}_i = \frac{\nu N}{N\rho} = \frac{\nu}{\rho} \Rightarrow \rho = \frac{\nu}{\sum_{i=1}^{N}\left(\frac{\tilde{\alpha}_i}{N\rho}\right)}.$$

Now, $\tilde{\alpha}_i/N\rho$ (as opposed to $\tilde{\alpha}_i$ or α_i) is the actual output of **NuSVC** and, since ν is user-defined, ρ is easily determined.

Note: If we should choose $\nu = 0$, we would have the condition $\sum_{i=1}^{N}\tilde{\alpha}_i = \nu N = 0$. Since each $\tilde{\alpha}_i$ is nonnegative, this means that all $\tilde{\alpha}_i = 0$. This is the *trivial* solution, and it implies that there are no support vectors at all. Hence, $\mathbf{w} = \mathbf{0}$ so that $b = 0$ and $\rho = 0$. Consequently, the discriminant for a test point $\mathbf{z}$ would be $\Delta\left(\boldsymbol{\varphi}(\mathbf{z})\middle|\mathbf{w},b\right) = \mathbf{w}\cdot\boldsymbol{\varphi}(\mathbf{z}) + b = 0$, so that all test points lie exactly on the decision surface. This is not useful, and so we must reject the trivial solution.

3 ν-SVC and C-SVC: A computational example

By way of an example for ν-SVC, we consider a dataset with $N = 1000$, $N_- = 200$ and $N_+ = 800$. So, in keeping with our established colour scheme, most of the data points are yellow, and the red points have been grouped into two clusters, as shown in the figures below.

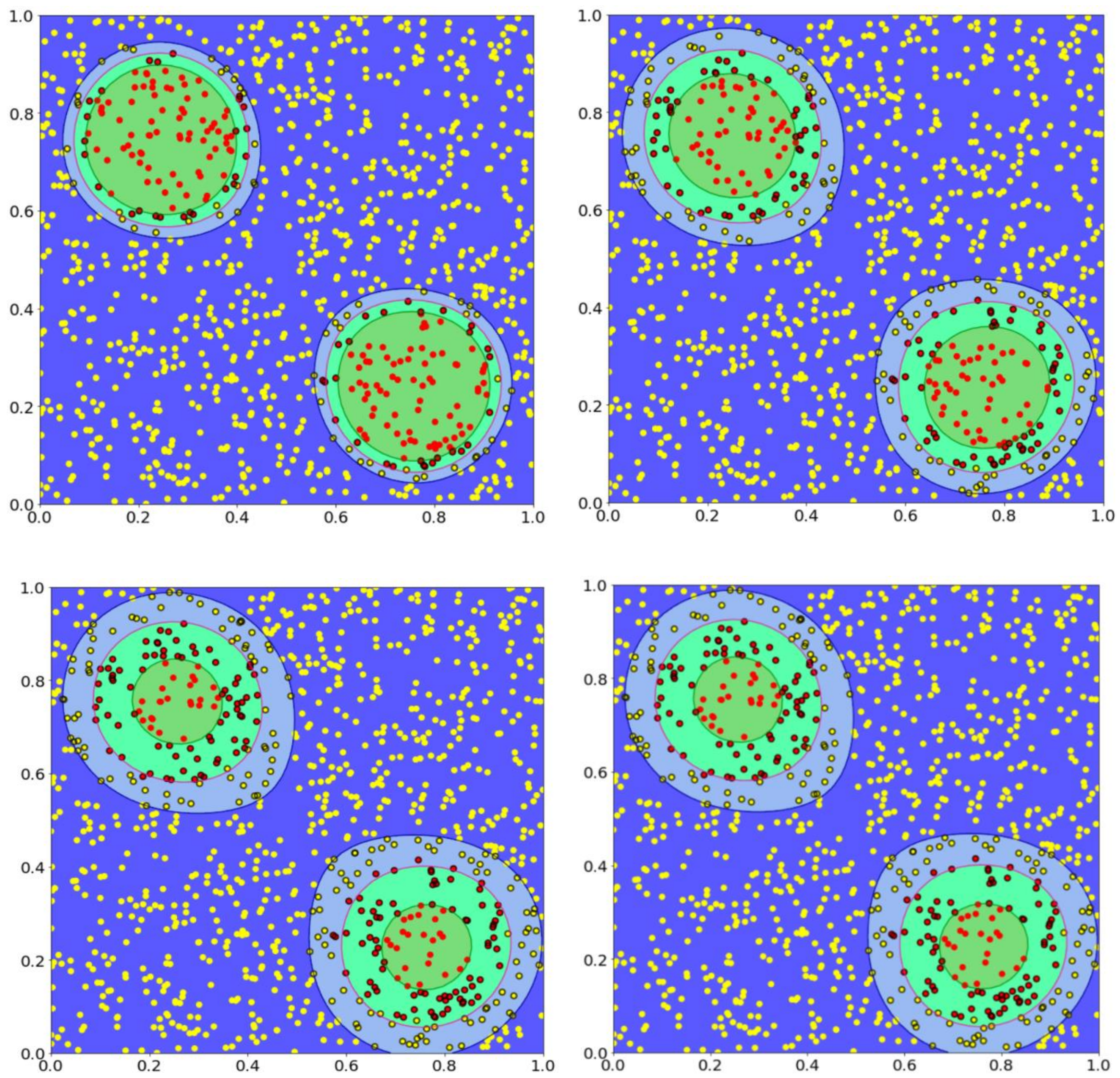

Figure 1: ν-SVC for various ν. C-SVC is lower right.

In this figure, solutions for the dataset using ν-SVC, with an RBF kernel, have been obtained, with $\nu = 0.1$ (upper left), $\nu = 0.2$ (upper right) and $\nu = 0.3$ (lower left). The lower right image shows a C-SVC solution with

$$C = \frac{1}{N\rho} = \frac{1}{(1000)(0.001746)} = 0.57289$$

where the value of ρ corresponds to the bottom left case. The parameter γ was fixed at $\gamma = 6$ for all computations. Clearly, the lower left and lower right solutions are identical.

We also see the effect of ν: as ν increases, the width of the margin increases. This is expected, since increasing ν raises the lower bound on the number of support vectors, and the margin width is increased to accommodate this bound. Indeed, the number of support vectors for the three values of ν considered here are 106, 207 and 305 – each of these is close to the bound νN. Note that there are a few incorrectly classified points in each case. Strictly speaking, the dataset was constructed to be separable in feature space. These misclassifications are due to the fact that we have allowed soft margins in the classifiers, and we have not attempted to optimize our choice of the hyperparameters C and γ.

These solutions also show the ability of the RBF kernel to find a sensible decision surface even though the red data points are separated into two 'islands' surrounded by the yellow points. Of course, what we see here is a 2D coloured pixel representation of the decision surface and the margin edges within the input space, whereas the actual computation was, in principle, performed in the infinite-dimensional feature space of the RBF kernel.

4 Deriving the primal from the dual

ν-SVC

The analysis for ν-SVC is similar to that for C-SVC [2] but involves a subtlety. Earlier (see p4), we derived the expression

$$\sum_{i=1}^{N} \alpha_i = \nu + \eta$$

from one of the stationarity conditions. Since $\eta \geq 0$ we clearly have

$$\sum_{i=1}^{N} \alpha_i \geq \nu.$$

This is the *general* form of this particular condition, and it is the form that we must use in this analysis – even though we previously replaced it with the more specific condition $\sum_{i=1}^{N} \alpha_i = \nu$.

So, we have

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

and the conditions

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

The Lagrangian is

$$L(\alpha,\zeta,b,\mu,\rho)=F_d+b\sum_{i=1}^{N}y_i\alpha_i-\sum_{i=1}^{N}\zeta_i\left(\frac{1}{N}-\alpha_i\right)-\sum_{i=1}^{N}\mu_i\alpha_i-\rho\left(\sum_{i=1}^{N}\alpha_i-\nu\right)$$

and its derivative is

$$\begin{aligned}\frac{\partial L}{\partial\alpha_i}&=\frac{\partial F_d}{\partial\alpha_i}+by_i+\zeta_i-\mu_i-\rho\\&=y_i\sum_{j=1}^{N}\alpha_j y_j K\left(\mathbf{x}_j,\mathbf{x}_i\right)+by_i+\zeta_i-\mu_i-\rho.\end{aligned}$$

Note that $\rho\geq 0$ since it is a KKT multiplier.

The stationarity condition gives

$$\frac{\partial L}{\partial\alpha_i}=y_i\sum_{j=1}^{N}\alpha_j y_j K\left(\mathbf{x}_j,\mathbf{x}_i\right)+by_i+\zeta_i-\mu_i-\rho=0$$

$$\Rightarrow\ y_i\left(\sum_{j=1}^{N}\alpha_j y_j K\left(\mathbf{x}_j,\mathbf{x}_i\right)+b\right)=\rho-\zeta_i+\mu_i$$

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

which are the primal conditions for ν-SVC .

The Lagrangian becomes

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

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

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

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

which finally gives

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

Observe that, by using the general form of the condition $\sum_{i=1}^{N}\alpha_i \geq \nu$, we have naturally found $\rho \geq 0$ and the correct sign in the term $-\rho\nu$. This would not have occurred if we had used the condition $\sum_{i=1}^{N}\alpha_i = \nu$. This is an equality condition and, as such, there would be no restriction on the sign of the multiplier ρ. Consequently, we would have had to artificially introduce a suitable sign restriction on ρ. This ambiguity is simply a consequence of a loss of information incurred when we modified the condition in our original derivation of the ν-SVC dual problem, from $\sum_{i=1}^{N}\alpha_i \geq \nu$ to $\sum_{i=1}^{N}\alpha_i = \nu$. The dual problem with $\sum_{i=1}^{N}\alpha_i = \nu$ is a perfectly valid problem but because it is not general, the ability to use it to regain the primal problem unambiguously is lost.

6 Concluding comments

We have provided mathematical detail pertaining to the soft-margin classifier ν-SVC, as used in **scikit-learn**. Further details regarding the SVC library in **scikit-learn**, as we understand them, can be found in [9].

Bibliography

We reproduce the bibliographies from [1, 2], with a few additional items of relevance.

1) J.S.C. Prentice, Support Vector Classifiers in scikit-learn: Mathematical Detail, Part I, *AfricArxiv Preprints*, 2023, (https://osf.io/preprints/africarxiv/4cj9w).
2) J.S.C. Prentice, Support Vector Classifiers in scikit-learn: Mathematical Detail, Part II, *AfricArxiv Preprints*, 2023, (https://osf.io/preprints/africarxiv/xnyem)
3) Bernhard E. Boser, Isabelle M. Guyon, Vladimir N. Vapnik, A Training Algorithm for Optimal Margin Classifiers*, Proceedings of the 5th Annual ACM Workshop on Computational Learning Theory*, 144–152 (1992).
4) C. Cortes, V. Vapnik, Support-Vector Networks, *Machine Learning*, 20, 273–297 (1995).
5) Bernhard Schölkopf, Robert Williamson, Alex Smola, John Shawe-Taylort, John Platt, Support Vector Method for Novelty Detection, *NIPS'99: Proceedings of the 12th International*

Conference on Neural Information Processing Systems, 582–588 (1999).

6) Koby Crammer, Yoram Singer, On the Algorithmic Implementation of Multiclass Kernel-based Vector Machines, *Journal of Machine Learning Research* 2, 265–292 (2001).
7) F. Pedregosa *et al.*, Scikit-learn: Machine Learning in Python, *Journal of Machine Learning Research*, 12, 2825–2830 (2011).
8) Chih-Wei Hsu, Chih-Chung Chang, and Chih-Jen Lin, A Practical Guide to Support Vector Classification, Technical report NTU, 2003 (original), 2016 (updated).
9) J.S.C. Prentice, *Support Vector Classifiers in scikit-learn*, eBook, Mathsophical, 2020, ISBN: 9780620910040 (This book is the primary source for the content of the paper).
10) Bernhard Schölkopf, Robert Williamson, Alex Smola, John Shawe-Taylort, John Platt, Support Vector Method for Novelty Detection, *NIPS'99: Proceedings of the 12th International Conference on Neural Information Processing Systems*, 582–588 (1999).
11) Bernhard Schölkopf, Robert C. Williamson, New Support Vector Algorithms, *Neural Computation* 12, 1207–1245 (2000).
12) Chih-Chung Chang, Chih-Jen Lin, Training ν-Support Vector Classifiers: Theory and Algorithms, *Neural Computation* 13, 2119–2147 (2001).
13) Pai-Hsuen Chen, Chih-Jen Lin and Bernhard Schölkopf, A tutorial on ν-support vector machines, *Appl. Stochastic Models Bus. Ind.*, 21, 111–136 (2005).

14) D. J. Crisp, C. J. C. Burges, *A Geometric Interpretation of ν-SVM Classifiers*, *Advances in Neural Information Processing Systems 12* (NIPS 1999).
15) Simon Haykin, *Neural Networks: A Comprehensive Foundation, 2nd ed.*, Prentice Hall, 1999, ISBN13: 9780132733502.
16) Christopher M. Bishop, *Pattern Recognition and Machine Learning*, Springer, 2006, ISBN13: 9780387310732.
17) T. Hastie, R. Tibshirani, J. Friedman, *The Elements of Statistical Learning: Data Mining, Inference, and Prediction, 2nd ed.*, Springer, 2009, ISBN13: 9780387848587.
18) Amnon Shashua, *Introduction to Machine Learning*, 2008, [arXiv:0904.3664v1].
19) S. Shalev-Shwartz, S. Ben-David, *Understanding Machine Learning: From Theory to Algorithms*, Cambridge University Press, 2014, ISBN13: 9781107057135.
20) Jake VanderPlas, *Python Data Science Handbook: Essential Tools for Working with Data*, O'Reilly, 2017, ISBN13: 9781491912058.
21) Nello Cristianini, John Shawe-Taylor, *An Introduction to Support Vector Machines and Other Kernel-based Learning Methods, 1st ed.*, Cambridge University Press, 2000, ISBN13: 9780521780193.
22) Bernhard Scholkopf, Alexander J. Smola, *Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond*, MIT Press, 2018, ISBN13: 9780262536578.

Appendix

Here, we provide the Python code that was used to generate the images in Figure 1. The classifiers C-SVC and ν-SVC are initialised in blocks 4 and 5. Values of γ, ν and C can be set in those blocks.

```
# Import the necessary packages
import numpy as np
from sklearn import svm
from sklearn.model_selection import GridSearchCV
import matplotlib.pyplot as plt
%matplotlib inline
```

```
# Define a dataset
# This dataset is two red clusters in a sea of yellow points
def trcisoy(N, radius2, seed):    # Define the function trcisoy that generates the dataset,
                                  # N=number of points overall, radius2=radius^2 of each red cluster,
                                  # seed=random seed
    np.random.seed(seed)

    X = np.r_[(np.random.rand(N, 2))]
    y = [1]*N
    y = np.array(y)

    XX = ((X[:,0]-0.25)**2+(X[:,1]-0.75)**2)
    index = np.where(XX<radius2)
    y[index[0]] = -1

    XX = ((X[:,0]-0.75)**2+(X[:,1]-0.25)**2)
    index = np.where(XX<radius2)
    y[index[0]] = -1
```

```
    X = X + (np.r_[(np.random.rand(N, 2))]-0.5)/10        # Add some random noise
    X = (X-X.min(axis=0))/(X.max(axis=0)-X.min(axis=0))   # Normalize to unit square

    return X, y
```

```
# Define a dataset using trcisoy
X, y = trcisoy(1000, 1/32, 80)
```

```
# Initialise a C-SVC classifier ………
classifier = svm.SVC(kernel='rbf', gamma=6, C=0.57289, class_weight={-1: 1, 1: 1}, tol=1e-12)
```

```
# ……… or initialise a nu-SVC classifier
#classifier = svm.NuSVC(kernel='rbf', gamma=6, nu=0.3, class_weight={-1: 1, 1: 1}, tol=1e-12)
```

```
# Fit the classifier
classifier.fit(X, y, sample_weight=np.ones(len(X)))
```

```
# Define some figure properties
plt.figure(figsize=(11,11))
plt.tick_params(axis='both', which='major', labelsize=20)
plt.tick_params(axis='both', which='minor', labelsize=8)
```

```
# Create xy grid
xx = np.linspace(0,1,50)
yy = np.linspace(0,1,50)
```

```
YY, XX = np.meshgrid(yy, xx)
xy = np.vstack([XX.ravel(), YY.ravel()]).T
```

```
# Determine the decision function
D = classifier.decision_function(xy).reshape(XX.shape)
```

```
# Plot decision boundary and margins
plt.contourf(XX, YY, D,  levels=[-1000,-1,0,1,1000],
colors=['limegreen','springgreen','cornflowerblue','blue'], alpha=0.65)
plt.contour(XX, YY, D, levels=[-1,0,1], colors=['green','deeppink','darkblue'], alpha=0.75)
```

```
# Plot data points and support vectors (s is divided by 4 if there are a large number of points -
# smaller dots improves clarity )
plt.scatter( X[:,0], X[:,1], c=y, s=200/4, alpha=1, cmap=plt.cm.autumn)
plt.scatter(classifier.support_vectors_[:,0], classifier.support_vectors_[:,1], s=200/4, alpha=0.75,
linewidth=2, facecolors='none', edgecolors='k')

plt.show()
```

This code was last run successfully on 20/8/2023 under Python `3.8.16` and **`scikit-learn`** `1.2.2`.