The soft-margin Support Vector Machine with ordered weighted average

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Abstract

This paper deals with an extension of the Support Vector Machine (SVM) for classification problems where, in addition to maximize the margin, i.e., the width of strip defined by the two supporting hyperplanes, the minimum of the ordered weighted sum of the deviations of misclassified individuals is considered. Since the ordered weighted sum includes as particular case the sum of these deviations, the classical SVM model is a particular case of the model under study. A quadratic continuous formulation for the case in which weights are sorted in non-decreasing order is introduced, and a mixed integer quadratic formulation for general weights is presented. In both cases, we show that these formulations allow us the use of kernel functions to construct non-linear classifiers. Besides, we report some computational results about the predictive performance of the introduced approach (also in its kernel version) in comparison with other SVM models existing in the literature.

Keywords: Data Science; Classification; Support Vector Machine; OWA Operators, Mixed Integer Quadratic Programming.

1 Introduction

Support Vector Machine (SVM) models have become one of the most used approaches of Mathematical Programming to address classification problems. SVM techniques have been applied in many different fields since the introduction of the classical soft margin SVM by Cortes and Vapnik (1995) and Vapnik (1998). Among
them, image recognition, bioinformatics, and face detection, see Cervantes et al. (2020) and references therein.

In the literature, many models based on the classical soft margin SVM approach have been developed with the aim of improving its predictive performance. For instance, different norms have been used to measure the margin between classes (Blanco et al., 2020b); outliers or label noise influence has been considered in some models (Baldomero-Naranjo et al., 2020, 2021; Blanco et al., 2020a); and other models also consider feature selection (Gaudioso et al., 2017; Jiménez-Cordero et al., 2021; Labbé et al., 2019; Lee et al., 2020; Maldonado et al., 2014).

In Maldonado et al. (2018) a new approach for the classical soft-margin Support Vector Machine is proposed. This methodology proposes to apply the OWA operator to modify the hinge loss function of classical SVM. The idea is rather appealing in that it allows to tune the importance of deviations according to their size. Thus, accounting differently classification errors with respect to a preference ranking induced by the sorting of their sizes (distances to the classification hyperplane).

The idea of penalizing the classification errors unevenly according to their sizes is aligned with the use of OWA operators that have become very popular in different areas of decision theory. Surprisingly, although very natural, this approach has been never tried in SVM and these authors propose a two-step heuristic method to solve their model: 1) the classical SVM is trained and its classification errors induce an order based on the distances to the classifier; 2) the SVM is re-trained using a weighted sum of classification errors with weights induced from the order of the solution in the first step. In Maldonado et al. (2020), they propose an analogous method, but using the induced order of fuzzy density-based methods for outlier detection. This approach is very simple and has the same complexity as the classical SVM beyond of being applied twice. Moreover, as the authors show in their paper, its predictive performance is superior to the traditional SVM in a set of databases that are reported in the paper.

We find the idea of applying OWA operators to classical SVM remarkable and we would like to contribute a bit more on it. Actually, our analysis shows that the approach by Maldonado et al. (2018) is a first step into this direction but it is not really an OWA operator. In fact, we think that there is still room for new contributions and improvements on this topic. Actually, we show in this paper that the methodology by Maldonado et al. (2018), denoted from now on as app-OWA-SVM, is a heuristic approximation to the exact application of OWA operators to classical SVM. Our aim with this paper is to develop the exact methodology for including OWA operators into SVM and to compare these results with classical SVM and with the approximated OWA version proposed by Maldonado et al. (2018).

Our contribution in this paper is the following. We present the exact application of OWA operators to the soft-margin hinge loss SVM and prove that the kernel extension of this methodology is also possible. Our analysis distinguishes between convex OWA operators (those induced by monotone non-decreasing weights) and non-convex ones. For the first family of methods the complexity of the exact OWA-SVM is similar to the classical SVM. However, the second family of methods,
namely the non-convex ones, is more complex in that it involves solving mixed-
exterior second-order cone programs. Yet, kernel transformations are also satisfac-
torily extended to this class and moreover, the resulting problems can be solved to
optimality with MIP-solvers such as Gurobi, Cplex or Xpress. We test the perfor-
mance of OWA-SVM compared with classical SVM and with app-OWA-SVM. Our
results confirm those already reported by Maldonado et al. (2018): OWA-SVM is
superior to SVM and it performs similarly to app-OWA-SVM. This last observation
shows that app-OWA-SVM provides good predictive performance similar to the one
of the exact OWA-SVM.

The remainder of this paper is structured as follows. In Section 2 some notation
and details about the problem are described. Section 3 is devoted to the develop-
ment of an SVM model which includes the OWA when non-decreasing weights are
considered. Besides, in Section 4 we introduce a general mixed integer quadratic
model which allows the use of the OWA for general weights (not necessarily non-
decreasing). Section 5 contains computational experiments carried out on several
datasets. Finally, Section 6 includes conclusions and some future research lines.

2 Soft margin hinge loss SVM including OWA operators

In binary classification problems, we are given a training set of individuals, \( N = \{1, \ldots, n\} \), divided into two classes. Each individual, \( i \), is represented by a pair
\((x_i, y_i) \in \mathbb{R}^d \times \{-1, 1\}\), where \( d \) is the number of considered features, \( x_i \) is a vector
with features’ values and \( y_i \) is the label associated with the class of the individual.
The goal of SVM models is to determine a hyperplane \( \mathbf{w}^T \mathbf{x} + b \) that optimally
separates the training set and that allows the classification of new individuals.

The classical soft margin SVM model is a compromise between maximizing the
distance (margin) between the two parallel class-supporting hyperplanes and min-
imizing the deviations of misclassified individuals. It is formulated as follows, see
Bradley and Mangasarian (1998),

\[
(\ell_2\text{-SVM}) \min_{w,b,\xi} \quad \frac{1}{2} \|w\|_2^2 + C \sum_{i=1}^{n} \xi_i,
\]

\[
\text{s.t.} \quad y_i(\mathbf{w}^T \mathbf{x}_i + b) \geq 1 - \xi_i, \quad i \in N, \\
\mathbf{w} \in \mathbb{R}^d, \\
b \in \mathbb{R}, \\
\xi_i \geq 0, \quad i \in N.
\]

In this formulation, \( w \)- and \( b \)-variables are the coefficients of the optimal separa-
tor hyperplane and \( \xi \)-variables represent the deviations associated with misclassified
individuals. The margin between both supporting hyperplanes is given by \( \frac{2}{\|w\|_2} \).

Consequently, as mentioned before, the objective function is a balance between the
maximization of the margin and the minimization of the deviations. Observe that this balance is regulated by the constant parameter $C$.

Non-linear classifiers can also be obtained by using the classical SVM model. In order to determine a non linear separator, data of the training set $N$ are mapped onto a higher dimension space by using a projection function $\phi(\cdot)$. By the use of duality theory and kernel functions, one can determine the optimal separator without explicitly knowing $\phi(\cdot)$. To clarify this aspect, it should be mentioned that kernel functions are those such that can be expressed as $K(x_i, x_j) = \phi(x_i) \cdot \phi(x_j)$, where $\cdot$ denotes the scalar product. This, together with the fact that dual formulation of $\ell_2$-SVM and the resulting optimal separating hyperplane only depend on the dot product of training samples, makes unnecessary the explicit use of $\phi(\cdot)$. For more details about this kernel-based method, see Burges (1998).

In the context of SVM models, OWA operators can be applied to the second term of the objective function of the classical SVM, i.e., considering the ordered weighted sum of deviations of misclassified individuals instead of the sum of them. The idea of OWA for a set of amounts is to consider the weighted sum of them but taking into account that the weights are assigned depending on the positions in the ordered sequence of these amounts. For instance, given a deviation vector $\xi'$, the ordered weighted sum of the components of this vector is $\sum_{i=1}^{n} \lambda_i \xi_{(i)}$. Where $\xi_{(1)}, \xi_{(2)}, \ldots, \xi_{(n)}$ is the vector $\xi'$ with its elements sorted in non-decreasing order and $\lambda_i \geq 0$ represents the weight associated with the $i$-th position of the ordered vector $\xi'$. Observe that for the case $\lambda_i = 1$, $\forall i \in N$, we obtain the sum of these amounts. Hence, a new SVM model considering OWA operator can be expressed as follows,

$$\min_{w, b, \xi} \frac{1}{2} \|w\|^2 + C \sum_{i=1}^{n} \lambda_i \xi_{(i)},$$

s.t. $\begin{align*}
y_i(w^T x_i + b) &\geq 1 - \xi_{i}, \quad i \in N, \\
\xi_{(i)} &\leq \xi_{(i+1)}, \quad i = 1, \ldots, n - 1, \\
w &\in \mathbb{R}^d, \\
b &\in \mathbb{R}, \\
\xi_i &\geq 0, \quad i \in N,
\end{align*}$

where $\xi_{(i)}$ is a variable that represents the $i$-th smallest deviation among the elements in the training set $N$. Note that elements of vector $\xi'$ are equal to the ones of $\xi$ but sorted in non-decreasing order.

In the next sections, we address the formulation of this problem. Recall that our objective is to provide an exact methodology for dealing with OWA operators with soft margin SVM. For this purpose, we distinguish between convex and non convex OWA operators. The reason of the aforementioned distinction is that, as we will detail in Section 3, the use of non-decreasing weights (convex case) allows to build a quadratic continuous formulation whose difficulty is similar to that of $\ell_2$-SVM. In contrast, the use of non-convex OWA operators leads to the introduction of a mixed
integer quadratic programming model which is computationally more complex. Section 4 deals with the use of these non-convex OWA operators. Besides, in sections 3 and 4, it will also be discussed if non-linear kernels can be accommodated in each model.

3 An SVM-model introducing convex OWA operators

In order to apply a correct OWA operator to the deviations of the SVM model, one has to multiply sorted deviation by the corresponding $\lambda$-weight in the formulation. We begin analyzing the case of monotone non-decreasing $\lambda$-weights since, as we will show, it induces simpler mathematical programming models.

With the aim of providing a formulation of this problem, together with the $w$, $b$, and $\xi$-variables used in the classical $\ell_2$-SVM, we need to include a new set of variables to model the order of the deviations of misclassified individuals. In particular, we define

$$z_{ij} = \begin{cases} 
1, & \text{if deviation of observation } i \text{ is in the } j\text{-th position of the sorted} \\
v \text{vector of deviations}, \\
0, & \text{otherwise},
\end{cases} \quad (1)$$

for $i, j \in N$. Given a vector of the deviation values related to each individual, $\xi^t$, the use of $z$-variables allows us to express the ordered weighted average of these deviations with $\lambda$-weights given in non-decreasing order as follows,

$$\sum_{i=1}^{n} \lambda_i \xi^t_{(i)} = \max_z \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_j \xi^t_{i} z_{ij},$$

subject to

$$\sum_{i=1}^{n} z_{ij} = 1, \quad j \in N, \quad (2)$$

$$\sum_{j=1}^{n} z_{ij} = 1, \quad i \in N, \quad (3)$$

$$z_{ij} \geq 0, \quad i, j \in N. \quad (4)$$

Constraints (2) and (3) ensure, respectively, that exactly one element of $N$ is in each position and that each position is allocated to exactly one element of $N$. Besides, due to total unimodularity property, $z$-variables can be relaxed as presented in (4). Hence, a formulation of the SVM with convex OWA operators is given by

$$\min_{w, b, \xi} \frac{1}{2} \|w\|^2_2 + \max_z \sum_{i=1}^{n} \sum_{j=1}^{n} C \lambda_j \xi_{i} z_{ij},$$

subject to

$$\text{(2) - (4)},$$

$$y_i (w^T x_i + b) \geq 1 - \xi_i, \quad i \in N, \quad (5)$$
\( w \in \mathbb{R}^d, \quad b \in \mathbb{R}, \quad \xi_i \geq 0, \quad i \in N. \)  

(6) \quad (7) \quad (8)

Like in the \( \ell_2 \)-SVM formulation, constraints (4) are the classical ones appearing in \( \ell_2 \)-SVM and the restrictions which determine the deviations of misclassified elements of \( N \). Constraints (6)-(8) determine the domains of the corresponding variables.

Observe that this optimization model includes an inner maximization problem which intends to obtain the OWA of deviations taking advantage of the fact of using a non-decreasing weight vector. Considering the results of Blanco et al. (2014) in the context of facility location problems, we obtain the following quadratic continuous formulation dualizing the inner problem.

\[
\text{(C-OWA-SVM)} \quad \min_{w,b,\xi,u,v} \quad \frac{1}{2} \|w\|^2 + \sum_{i=1}^{n} u_i + \sum_{j=1}^{n} v_j, \\
\text{s.t.} \quad (5), (6)-(8), \\
\quad u_i + v_j \geq C \lambda_j \xi_i, \quad j \in N, \quad (9) \\
\quad u_i \in \mathbb{R}, \quad i \in N, \quad (10) \\
\quad v_j \in \mathbb{R}, \quad j \in N. \quad (11)
\]

Where \( v \)- and \( u \)-variables are dual variables associated with constraints (2) and (3), respectively. Note that C-OWA-SVM is a quadratic continuous model which determines a linear classifier considering ordered weighted average of individuals errors.

**Remark 3.1** By considering the model proposed in Ogryczak and Tamir (2003) for minimizing the sum of \( k \) largest functions, an alternative formulation to C-OWA-SVM is

\[
\text{(OT-C-OWA-SVM)} \quad \min_{w,b,\xi,t,d} \quad \frac{1}{2} \|w\|^2 + \sum_{k=1}^{n} (\lambda_{n-k+1} - \lambda_{n-k}) \left( k t_k + \sum_{i=1}^{n} d_{ik} \right), \\
\text{s.t.} \quad (5), (6)-(8), \\
\quad d_{ik} \geq C \xi_i - t_k, \quad i, k \in N, \quad (i) \\
\quad d_{ik} \geq 0, \quad i, k \in N, \quad (ii) \\
\quad t_k \in \mathbb{R}, \quad k \in N. \quad (iii)
\]

Some preliminary computational results show that formulation C-OWA-SVM outperforms, in terms of computational times, formulation OT-C-OWA-SVM.

As in classical SVM, it would be interesting to check whether it is possible to develop a methodology for obtaining non-linear separators by applying the kernel
trick. For this reason, once we have a primal formulation of C-OWA-SVM, we present its dual version that will be very useful to build non linear classifiers. The following results give a formulation of the dual problem.

**Proposition 3.1** The dual form of C-OWA-SVM is given by:

$$
\begin{align*}
\max_{\alpha, \eta} & \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j x_i \cdot x_j, \\
\text{s.t.} & \quad \sum_{i=1}^{n} \alpha_i y_i = 0, \quad (12) \\
& \quad \alpha_i \leq \sum_{j=1}^{n} \eta_{ij} C \lambda_j, \quad i \in N, \quad (13) \\
& \quad \sum_{i=1}^{n} \eta_{ij} = 1, \quad j \in N, \quad (14) \\
& \quad \sum_{j=1}^{n} \eta_{ij} = 1, \quad i \in N, \quad (15) \\
& \quad 0 \leq \alpha_i, \quad i \in N, \quad (16) \\
& \quad 0 \leq \eta_{ij}, \quad i, j \in N. \quad (17)
\end{align*}
$$

**Proof:** The Lagrangian function associated with model C-OWA-SVM is

$$
L(w, b, \xi, u, v) = \frac{1}{2} \|w\|^2 + \sum_{i=1}^{n} u_i + \sum_{j=1}^{n} v_j + \sum_{i=1}^{n} \alpha_i [1 - \xi_i - y_i (w^T x_i + b)] \\
- \sum_{i=1}^{n} \mu_i \xi_i + \sum_{i=1}^{n} \sum_{j=1}^{n} \eta_{ij} (C \lambda_j \xi_i - u_i - v_j),
$$

where $\alpha \geq 0$, $\mu \geq 0$ and $\eta \geq 0$ are positive Lagrangian multipliers. The necessary and sufficient optimality conditions for C-OWA-SVM result in:

$$
\begin{align*}
\frac{\partial L(w, b, \xi, u, v)}{\partial w_j} &= w_j - \sum_{i=1}^{n} \alpha_i y_i x_{ij} = 0, \quad j \in N, \quad (18) \\
\frac{\partial L(w, b, \xi, u, v)}{\partial b} &= - \sum_{i=1}^{n} \alpha_i y_i = 0, \quad (19) \\
\frac{\partial L(w, b, \xi, u, v)}{\partial \xi_i} &= -\alpha_i - \mu_i + \sum_{j=1}^{n} \eta_{ij} C \lambda_j = 0, \quad i \in N, \quad (20)
\end{align*}
$$
\[ \frac{\partial L(w, b, \xi, u, v)}{\partial u_i} = 1 - \sum_{j=1}^{n} \eta_{ij} = 0, \quad i \in N, \quad (21) \]

\[ \frac{\partial L(w, b, \xi, u, v)}{\partial v_j} = 1 - \sum_{i=1}^{n} \eta_{ij} = 0, \quad j \in N, \quad (22) \]

\[ \alpha_i [1 - \xi_i - y_i (w^T x_i + b)] = 0, \quad i \in N, \quad (23) \]

\[ \mu_i \xi_i = 0, \quad i \in N, \quad (24) \]

\[ \eta_{ij} (C \lambda_j \xi_i - u_i - v_j) = 0, \quad i, j \in N, \quad (25) \]

\[ \alpha_i, \mu_i, \eta_{ij} \geq 0, \quad i, j \in N. \quad (26) \]

From (18), it can be shown that \( w_j = \sum_{i=1}^{n} \alpha_i y_i x_{ij} \) for \( j \in N \). Besides, as in the classic SVM, condition (19) results in constraint (12). In addition, conditions (20) can be replaced by inequalities (13). Finally, constraints (21) and (22) can be deduced from conditions (21) and (22), respectively.

By using the complementary slackness conditions and replacing \( w_j = \sum_{i=1}^{n} \alpha_i y_i x_{ij} \) in the Lagrangian function, we obtain

\[ L(w, b, \xi, u, v) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j x_i \cdot x_j. \]

\[ \square \]

Observe that the formulation of the dual problem depends on the observed data through the scalar product of two observations. Hence, replacing in C-OWA-SVM the scalar products of training data by a kernel function \( K(x_i, x_j) = \phi(x_i) \cdot \phi(x_j) \), where \( \phi \) is a map of the observations in a higher dimension space, the resulting formulation is

\[ \text{(C-OWA-SVM}_K) \max_{\alpha, \eta} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K(x_i, x_j), \]

\[ \text{s.t.} \quad (12) - (17). \]

Thus, kernel trick can be applied. Recall that this trick consists in using kernel functions in such a way that it is not necessary to explicitly know the transformation \( \phi(\cdot) \) and this formulation does not depend on the dimension of feature space.

Given a sample, \( x \), belonging to an unknown class, the separator function of a non linear SVM is given by

\[ w^T \phi(x) + b = \sum_{i=1}^{n} \alpha_i^* y_i \phi(x_i) \cdot \phi(x) + b = \sum_{i=1}^{n} \alpha_i^* y_i K(x_i, x) + b. \quad (27) \]

When using C-OWA-SVM\(_K \) to obtain a non linear separator, \( \alpha^* \) values are given by the optimal solution of C-OWA-SVM\(_K \). The following result states how to determine the value of \( b \) coefficient.

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Proposition 3.2 \( b \)-coefficient of the separator function associated with C-OWA-SVM is given by
\[
b = 1 - y_k \left( \sum_{i=1}^{n} \alpha_i y_i K(x_i, x_k) \right) \left/ \frac{y_k}{y_k} \right.,
\]
where \( k \in \mathbb{N} \) verifies that \( 0 < \alpha^*_k < C \sum_{j=1}^{n} \eta^*_{kj} \lambda_j \), and \((\alpha^*, \eta^*)\) are the optimal values of C-OWA-SVM\(_K\).

**Proof:** Let \( k \in \mathbb{N} \) be such that \( 0 < \alpha^*_k < C \sum_{j=1}^{n} \eta^*_{kj} \lambda_j \). Then, due to conditions (20), \( \mu^*_k > 0 \). Since (24) holds, \( \xi^*_k = 0 \). Considering (23), we obtain
\[
1 - y_k \left( \sum_{i=1}^{n} \alpha_i y_i K(x_i, x_k) + b \right) = 0.
\]
Then,
\[
b = 1 - y_k \left( \sum_{i=1}^{n} \alpha_i y_i K(x_i, x_k) \right) \left/ y_k \right.
\]
\[\square\]

The discussion above proves that kernel trick can be used in OWA-SVM provided that \( \lambda \)-weights are given in non-decreasing order and that C-OWA-SVM\(_K\) formulation is used. Furthermore, the non linear separator can be easily obtained by using (27) and Proposition 3.2.

Regarding formulation C-OWA-SVM\(_K\), we find some differences with respect to the classical kernel extension of \( \ell_2 \)-SVM. Specifically, it is necessary to include some variables \((\eta)\) and constraints ((13)-(15),(17)) which do not appear in the classical dual model. Despite this, the resulting formulation C-OWA-SVM\(_K\) is a convex quadratic continuous formulation that can be solved in reasonable small times comparable to the times of classical kernel-version SVM model as we will see in Section 5. Then, we have obtained an exact OWA-SVM approach for non-decreasing \( \lambda \)-weights that can be efficiently solved.

4 An SVM-model introducing non convex OWA operators

The main goal of this Section is to introduce OWA in the SVM model when general \( \lambda \)-weights are considered, not necessarily given in non decreasing order. In contrast with the formulation addressed in the previous section, the use of general \( \lambda \)-weights forces the introduction of binary variables in the formulation in order to model the sorting of the SVM related deviations. As a consequence, the resulting model is a quadratic mixed integer formulation which is computationally more complex than C-OWA-SVM. Besides, in spite of using a MIQP to model OWA-SVM with general \( \lambda \)-weights, we are able to deal with a kernel extension in a different way.
As previously mentioned, OWA operators with general \( \lambda \)-weights have been applied in many combinatorial optimization problems. Particularly, in Fernández et al. (2014), OWA problems are analyzed from a modeling point of view and several formulations are compared. Based on this analysis, we present a quadratic mixed integer formulation for the SVM model that we are studying.

To this purpose, it is necessary to use the \( z \)-variables described in (1) and to introduce a new family of continuous variables, for \( k \in N \), defined as:

\[
\theta_k = \text{deviation associated with the individual which is in the } k\text{-th position of the sorted vector of deviations,}
\]

The resulting formulation is the following:

\[
\text{(NC-OWA-SVM)} \quad \min_{w, b, \xi, z, \theta} \quad \frac{1}{2} \|w\|^2_2 + C \sum_{k=1}^{n} \lambda_k \theta_k,
\]

s.t. \( (5), (2), (6) - (8), (30) \),

\[
\theta_k \geq \xi_i - M (1 - \sum_{j=1}^{n} z_{ij}), \quad i, k \in N, \tag{28}
\]

\[
z_{ik} \in \{0, 1\}, \quad i, k \in N, \tag{29}
\]

\[
\theta_k \geq 0, \quad k \in N. \tag{30}
\]

Constraints (28) ensure that deviation value in position \( k \) is at least the deviation of element \( i \), if \( i \) is in a position smaller than or equal to \( k \), for \( i, k \in N \). Constraints (28) use a big \( M \) parameter to establish this link between \( \theta_k \)- and \( \xi_i \)-variables. Note that the maximum distance between two points of the training data is a valid value of \( M \).

Observe that, in contrast with formulation C-OWA-SVM, it is necessary to include binary variables to correctly model the order. As a consequence, completely different techniques must be applied to extend kernel trick to this formulation. In what follows, we develop a model to accommodate non linear kernel functions in NC-OWA-SVM, see Brooks (2011).

**Remark 4.1** In model NC-OWA-SVM, assume that \( z \)-variables are fixed to \( \hat{z} \) (feasible assignment). Then the following formulation can be stated,

\[
\text{(NC-OWA-SVM(\hat{z}))} \quad \min_{w, b, \xi, \theta} \quad \frac{1}{2} \|w\|^2_2 + C \sum_{k=1}^{n} \lambda_k \theta_k,
\]

s.t. \( (5), (6) - (8), (20) \),

\[
\theta_k \geq \xi_i - M (1 - \sum_{j=1}^{n} \hat{z}_{ij}), \quad i, k \in N. \tag{31}
\]
The dual formulation of NC-OWA-SVM($\hat{z}$) is

$$
(NC\text{-}OWA\text{-}SVM_D(\hat{z})) \max_{\alpha, \mu} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j \quad \text{s.t. (12), (16), (32)}
$$

$$
- M \sum_{i=1}^{n} \sum_{k=1}^{n} \mu_{ik} \left(1 - \sum_{j \leq k} \hat{z}_{ij}\right),
$$

$$
\alpha_i \leq \sum_{k=1}^{n} \mu_{ik}, \quad i \in N; \quad \sum_{i=1}^{n} \mu_{ik} \leq C \lambda_k, \quad i, k \in N; \quad \mu_{ik} \geq 0, \quad i, k \in N.
$$

Besides, from necessary and sufficient optimality conditions, $w_j = \sum_{i=1}^{n} \alpha_i y_i x_{ij}$ for $j \in N$.

Based on the link between NC-OWA-SVM($\hat{z}$) and NC-OWA-SVM$_D(\hat{z})$, we propose an alternative formulation of OWA-SVM for general weights. This formulation allows the use of kernel functions, and consequently, the use of non-linear separators.

$$(NC\text{-}OWA\text{-}SVM_D) \min_{\alpha, \theta, \xi, b, z} \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j \mathbf{x}_i \cdot \mathbf{x}_j + C \sum_{k=1}^{n} \lambda_k \theta_k,$$

$$\text{s.t. (2), (7), (8), (28) - (30)},$$

$$
y_i \left(\sum_{j=1}^{n} y_j \alpha_j \mathbf{x}_i \cdot \mathbf{x}_j + b\right) \geq 1 - \xi_i, \quad i \in N.
$$

**Proposition 4.1** Given an optimal solution of NC-OWA-SVM, $(w^*, \theta^*, \xi^*, \theta^*, z^*)$, it can be built a feasible solution of NC-OWA-SVM$_D$, $(\alpha^*, b^*, \xi^*, \theta^*, z^*)$, with the same objective value.

**Proof:**

Given a solution of NC-OWA-SVM, $(w^*, \theta^*, \xi^*, \theta^*, z^*)$, then $(w^*, \theta^*, \xi^*, \theta^*)$ is an optimal solution of NC-OWA-SVM$_D(z^*)$. From necessary and sufficient optimality conditions, $w^* = \sum_{i=1}^{n} \alpha'_i y_i x_{ij}$, where $\alpha'$ are the optimal values of $\alpha$ variables appearing in NC-OWA-SVM$_D(z^*)$. By defining $\alpha^* = \alpha'$, $(\alpha^*, b^*, \xi^*, \theta^*, z^*)$ is feasible for NC-OWA-SVM$_D$ and
\[
\frac{1}{2} \| w^* \|^2_2 + C \sum_{k=1}^{n} \lambda_k \theta_k^* = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i^* \alpha_j^* x_i \cdot x_j + C \sum_{k=1}^{n} \lambda_k \theta_k^*.
\]

**Proposition 4.2**  Given an optimal solution of NC-OWA-SVM\(_D\), \((\alpha^*, b^*, \xi^*, \theta^*, z^*)\), a feasible solution of NC-OWA-SVM with the same objective value, \((w^*, b^*, \xi^*, \theta^*, z^*)\), can be built.

**Proof:**

Given an optimal solution of NC-OWA-SVM\(_D\), \((\alpha^*, b^*, \xi^*, \theta^*, z^*)\), we define 
\[w_j^* = \sum_{i=1}^{n} \alpha_i^* y_i x_{ij} \] 
This solution is feasible for NC-OWA-SVM since NC-OWA-SVM\(_D\) has been built from NC-OWA-SVM, by replacing 
\[w_j \] 
by \[\sum_{i=1}^{n} \alpha_i y_i x_{ij} \].

\[\Box\]

Propositions 4.1 and 4.2 show that formulations NC-OWA-SVM and NC-OWA-SVM\(_D\) are equivalent in the sense that optimal solutions to NC-OWA-SVM can be built from optimal solutions of NC-OWA-SVM\(_D\) with the same objective value, and vice versa. Note that formulation NC-OWA-SVM\(_D\) allows us to accommodate non linear kernel functions. Replacing scalar products by a general kernel function, the resulting formulation is

\[\text{(NC-OWA-SVM\(_K\))} \quad \min_{\alpha, b, \xi, \theta, z} \quad \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j K(x_i, x_j) + C \sum_{k=1}^{n} \lambda_k \theta_k,\]

\[\text{s.t.} \quad \begin{align*}
(2), (7), (38) - (39), \\
y_i \left( \sum_{j=1}^{n} y_j \alpha_j K(x_i, x_j) + b \right) &\geq 1 - \xi_i, \quad i \in N. \quad (36)
\end{align*}\]

Observe that, in NC-OWA-SVM\(_K\) formulation, a valid value for big \(M\) parameter should be determined and, the tighter the formulation, the better the performance. In order to obtain a good estimate for \(M\), one can solve the following auxiliary problem:

\[\text{(UBM)} \quad \max_{\alpha, b, \xi, \theta} \quad \theta,\]

\[\text{s.t.} \quad \begin{align*}
(7), (38), (39), (40), \\
\theta &\geq \xi_i, \quad i \in N \quad (37) \\
\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j K(x_i, x_j) + C \lambda_\theta \theta &\leq \text{UB}, \quad i \in N \quad (38) \\
0 &\leq \alpha_i \leq C \sum_k \lambda_k, \quad i \in N, \quad (39)
\end{align*}\]
\[
\theta \geq 0, \tag{40}
\]

where UB is an upper bound on the optimal value of NC-OWA-SVM\(_K\) and \(\theta\) is a variable that represents the deviation of the individual that is in the \(n\)-th position of the sorted vector of deviations, the largest one. In UB\(_M\) formulation, constraint (12) must be satisfied since it appears in NC-OWA-SVM\(_D(z')\) for each feasible assignment \(z'\). In addition, constraints (36) ensure that \(\alpha\) solutions satisfy the constraints of NC-OWA-SVM\(_K\) and constraints (37) establish that \(\theta\) is the largest deviation. Besides, we include constraint (35) which restrict the objective value of the original problem to be smaller than or equal to a certain upper bound. Finally, the remaining constraints determine the bounds of the problem variables. Note that constraints (39) result from the combination of constraints (32) and (33) appearing in formulation NC-OWA-SVM\(_D(z)\).

In a similar way, upper and lower bounds on \(b\)-variable could be obtained. Particularly,

\[
(UB_b) \quad \max_{\alpha, b, \xi, \theta} \quad b, \\
\text{s.t.} \quad (7), (8), (12), (36) - (40)
\]

provides an upper bound on \(b\)-variable. Analogously,

\[
(LB_b) \quad \min_{\alpha, b, \xi, \theta} \quad b, \\
\text{s.t.} \quad (7), (8), (12), (36) - (40)
\]

allows us to obtain a lower bound on \(b\)-variable.

We can conclude that, by using an initial upper bound on C-OWA-SVM\(_K\) (UB), and auxiliary problems (UB\(_M\), UB\(_b\), LB\(_b\)), a valid \(M\) value and bounds on the \(b\)-variable can be determined. Then, NC-OWA-SVM\(_K\) can be solved more efficiently. In Algorithm 1 the method for solving NC-OWA-SVM\(_K\) is outlined.

Next section will be devoted to some computational studies on the different OWA-SVM models.

5 Computational experiments

As mentioned in the Introduction, Maldonado et al. (2018) present a heuristic approach to the use of OWA in the soft-margin SVM, that for the sake of presentation we denote by app-OWA-SVM. The app-OWA-SVM approach is a two-step method. In the first step, the classical soft margin SVM is solved and in the second step, the order induced by this optimal solution on the deviations is used to assign fixed weights to a new soft-margin SVM model.

In this Section, we analyze the performance of our exact approach to OWA-SVM in comparison with app-OWA-SVM and the classical soft-margin SVM. These methods are applied to the six datasets described in Table 1 taken from UCI repository,
Algorithm 1: Method for solving NC-OWA-SVM$_K$.

**Data:** Training sample composed by a set of $n$ individuals with $d$ features.

**Result:** OWA-SVM classifier using non convex weights and a certain kernel function $K(\cdot, \cdot)$.

1. Solve the dual form of problem $\ell_2$-SVM with kernel function $K(\cdot, \cdot)$ obtaining a solution $(\alpha', b')$.

2. Consider the deviations associated with the optimal solution $(\alpha', b')$ and sort them in non-decreasing order, obtaining a sorted vector of deviations $\theta'$.

3. Build a feasible solution for NC-OWA-SVM$_K$:

$$UB^* := \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i' \alpha_j' K(x_i, x_j) + C \sum_{k=1}^{n} \lambda_k \theta_k'$$

4. Solve the problems $LB_b$ and $UB_b$ establishing $UB=UB^*$ in constraints (38). Obtain optimal objective values: $l_b$ from $LB_b$ and $u_b$ from $UB_b$.

5. Solve the problem $UB_M$ establishing $UB=UB^*$ in constraints (38) and adding constraint:

$$l_b \leq b \leq u_b. \quad (41)$$

The optimal solution of $UB_M$ is denoted as $ub_M$.

6. Solve NC-OWA-SVM$_K$ including constraints (38) and using $M = ub_M$. The optimal solutions of NC-OWA-SVM$_K$ are denoted by $(\alpha^*, b^*, \xi^*, \theta^*, z^*)$.
see Asuncion and Newman (2007). Actually, these datasets were the ones used by Maldonado et al. (2018) to check the validity of their approach, app-OWA-SVM. Observe that Table 1 details the complete names of the datasets, the sample size, the number of features and the proportion of each class in the sample.

| Label | Complete name         | n   | d   | Class(%)  |
|-------|-----------------------|-----|-----|-----------|
| IONO  | Ionosphere            | 351 | 34  | 64.1/35.9 |
| WBC   | Wisconsin Breast Cancer | 569 | 30  | 62.7/37.3 |
| AUS   | Australian Credit     | 690 | 14  | 55.5/44.5 |
| DIA   | Pima Indians Diabetes | 768 | 8   | 65.1/34.9 |
| GC    | German Credit         | 1000| 24  | 70.0/30.0 |
| SPL   | Splice                | 1000| 60  | 51.7/48.3 |

Table 1: Analyzed datasets from UCI repository

Our comparison not only includes the previously mentioned models using linear kernel, but also the influence of Gaussian kernel. Recall that the Gaussian kernel function can be expressed as

$$K(x_i, x_j) = \exp\left (-\frac{\|x_i - x_j\|^2}{2\sigma^2} \right ),$$

where $\sigma > 0$ is known as the width parameter, see Schölkopf and Smola (2002). For that reason, in the reported results, we distinguish between the results of the model with and without the Gaussian kernel.

In order to define the parameters, we follow the same strategy as in Maldonado et al. (2018). Specifically, we performed a ten fold cross validation for $C$ and $\sigma$ in $\{2^{-7}, 2^{-6}, \ldots, 2^6, 2^7\}$.

Moreover, we analyze four OWA weights based on linguistic quantifiers (see Luukka and Kurama (2013); Yager (1988)): basic, quadratic, exponential and trigonometric. For the sake of completeness, we recall the expressions of these quantifiers:

- Basic quantifier: $Q_b(r) = r^{\tilde{\alpha}}$, $\tilde{\alpha} \geq 0$.
- Quadratic quantifier: $Q_q(r) = \left ( \frac{1}{1 - \tilde{\alpha}(r)^{0.5}} \right )$, $\tilde{\alpha} \geq 0$.
- Exponential quantifier: $Q_e(r) = e^{-\tilde{\alpha}r}$, $\tilde{\alpha} \geq 0$.
- Trigonometric quantifier: $Q_t(r) = \arcsin(r\tilde{\alpha})$, $\tilde{\alpha} \geq 0$.

Considering these quantifiers, the associated weights can be determined by calculating

$$\lambda'_i = Q\left (1 - \frac{i - 1}{n}\right ) - Q\left (1 - \frac{i}{n}\right ), \text{ for } i \in N.$$

Hence, the final weights are given by

$$\lambda_i = \frac{\lambda'_i}{\lambda'}.$$
where $\bar{\lambda}'$ is the average of $\lambda'$-vector.

The specific choice of these weights is motivated since they are the ones reported in Maldonado et al. (2018). Note that the quantifiers related to the weights include a new parameter $\tilde{\alpha}$ which is also validated in $\tilde{\alpha} \in \{0.2, 0.4, 0.6, 0.8\}$.

To compare the results of the models, two classification performance metrics are presented: the accuracy (ACC) and the area under the curve (AUC). The accuracy is calculated as

$$\text{ACC} = \frac{TP + TN}{TP + TN + FP + FN},$$

where TP are true positives, TN are true negatives, FP false positives and FN false negatives. The area under the curve is given by

$$\text{AUC} = \frac{TP}{TP + FN} + \frac{TN}{TN + FP}.\frac{1}{2}.$$

Regarding the solution methods used for solving the models, classical soft-margin $\ell_2$-SVM and the $\ell_2$-SVM model using Gaussian kernel are solved with SVC function of Scikit Learn module in Python, see Pedregosa et al. (2011). Moreover, app-OWA-SVM and app-OWA-SVM$_K$, the models with linear and Gaussian kernel (respectively) appearing in Maldonado et al. (2018) are solved by using the two-step method proposed by them.

The exact OWA-SVM models that we propose can be solved depending on the weights with different approaches. Specifically, C-OWA-SVM$_K$ is used for the weights based on basic and exponential quantifiers since they are monotone non-decreasing. Besides, the weight based on the quadratic quantifier is also monotone non-decreasing for $\tilde{\alpha} = 0.2$. For this reason, C-OWA-SVM$_K$ is also used with these weights. Note that C-OWA-SVM$_K$ formulation is also the one used in the linear kernel case, i.e., $K(x_i, x_j) = x_i \cdot x_j$. For the remaining weights, NC-OWA-SVM and NC-OWA-SVM$_K$ (following Algorithm I) are applied to obtain the classifiers. It should be noted that all our computational studies were performed using CPLEX 20.1.0 in Python on an Intel(R) Xeon(R) W-2245 CPU 256 GB RAM computer.

Before comparing the predictive performance of the models, we would like to emphasize the level of adequacy provided by app-OWA-SVM with respect to the correct final ranking of the deviations. Table 2 reports an illustrative example of how the order of deviations behave in app-OWA-SVM methods compared with the correct final ranking. Specifically, Table 2 reports, for the considered datasets, the average percentage of coincidences between the positions that occupy the individuals in the sorted deviations vector of step one and their positions in step two of the app-OWA-SVM method. In addition, in the third column of Table 2 we report the average percentage of coincidences between the final order in the app-OWA-SVM method and the order provided by C-OWA-SVM$_K$. It should be highlighted that these results are obtained when applying the ten fold cross validation to the models with $C = 1$, $\sigma = 1$, basic quantifier weight, and $\tilde{\alpha} = 0.6$. 

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Results of Table 2 show how the induced order of classical SVM, in step 1 in Maldonado et al. (2018), is not the same as the one resulting in the second step of app-OWA-SVM. This order is neither the same as the sorting obtained by applying C-OWA-SVM\(K\). In contrast with the approaches in Maldonado et al. (2018), the exact OWA-SVM models, proposed in this paper, set the order of the deviations while solving the model itself and therefore they actually apply exact OWA operators to SVM. This shows that the method in Maldonado et al. (2018) is a OWA-like approach but actually, it is not an exact application of OWA operators.

| Data | Step 1 - Step 2 (%) | Step 2 - C-OWA-SVM\(K\) (%) |
|------|---------------------|-----------------------------|
| IONO | 1.68%               | 2.06%                       |
| WBC  | 1.17%               | 0.18%                       |
| AUS  | 0.86%               | 1.71%                       |
| DIA  | 0.56%               | 1.62%                       |
| GC   | 0.40%               | 0.36%                       |
| SPL  | 0.03%               | 0.00%                       |

Table 2: Average percentage of coincidence in the positions of the sorted deviations vector

Focusing on the performance classification metrics, Table 3 reports the best results in terms of ACC provided by the different models. Note that \(\ell_2\)-SVM and \(\ell_2\)-SVM\(K\) show the ACC of the classic model with linear and Gaussian kernels, respectively. The column corresponding to app-OWA-SVM presents the results of the model proposed in Maldonado et al. (2018) and column app-OWA-SVM\(K\) shows the results for the model in Maldonado et al. (2018) using the Gaussian kernel. Finally, ex-OWA-SVM and ex-OWA-SVM\(K\) report the best results of our proposed exact OWA-SVM methods using the formulations in sections 3 and 4. Observe that, for all datasets, the best ACC are either the one provided by the method presented in Maldonado et al. (2018) using the Gaussian kernel, or the ACC of the exact OWA-SVM model using the Gaussian kernel.

Particularly, ex-OWA-SVM\(K\) provides the best ACC results for WBC and AUS datasets; app-OWA-SVM\(K\) and ex-OWA-SVM\(K\) seem to yield the same results in the IONO and GC cases; whereas the best results for DIA and SPL are obtained by app-OWA-SVM\(K\). In general, we can observe that the accuracy (ACC) of app-OWA-SVM\(K\) and ex-OWA-SVM\(K\) are similar. This indicates that both approaches are worthy in the sense that they improve this classification performance metric with respect to the classical SVM achieving almost the same value.

Table 4 reports the AUC for the best combination of parameter values in each case. As for the ACC measure, the best AUC results are always provided by app-OWA-SVM\(K\) and ex-OWA-SVM\(K\). Regarding the results, we observe that the AUC of both approaches are quite similar. For the IONO, DIA and SPL datasets, the same AUC is achieved by app-OWA-SVM\(K\) and ex-OWA-SVM\(K\); ex-OWA-SVM\(K\) provides the best results for the WBC and AUS datasets; and finally, the app-
### Table 3: Best ACC results of each model

| Data | $\ell_2$-SVM | app-OWA-SVM | ex-OWA-SVM | $\ell_2$-SVM$_K$ | app-OWA-SVM$_K$ | ex-OWA-SVM$_K$ |
|------|--------------|-------------|------------|-----------------|----------------|----------------|
| IONO | 90.60%       | 90.89%      | 90.89%     | 95.44%          | 95.72%         | 95.72%         |
| WBC  | 98.07%       | 98.67%      | 97.71%     | 98.24%          | 98.42%         | 98.77%         |
| AUS  | 85.51%       | 86.09%      | 85.51%     | 86.38%          | 87.25%         | 87.39%         |
| DIA  | 77.60%       | 77.73%      | 77.73%     | 77.34%          | 78.38%         | 78.12%         |
| GC   | 76.90%       | 77.50%      | 77.30%     | 77.30%          | 77.50%         | 77.50%         |
| SPL  | 81.30%       | 82.00%      | 81.70%     | 88.40%          | 89.80%         | 89.40%         |

OWA-SVM$_K$ reports the best values of AUC for GC dataset. Both approaches, app-OWA-SVM$_K$ and ex-OWA-SVM$_K$, improve the AUC of the classical $\ell_2$-SVM and $\ell_2$-SVM$_K$.

### Table 4: Best AUC results for each model

| Data | $\ell_2$-SVM | app-OWA-SVM | ex-OWA-SVM | $\ell_2$-SVM$_K$ | app-OWA-SVM$_K$ | ex-OWA-SVM$_K$ |
|------|--------------|-------------|------------|-----------------|----------------|----------------|
| IONO | 88.67%       | 88.89%      | 88.89%     | 94.55%          | 95.15%         | 95.15%         |
| WBC  | 97.70%       | 97.70%      | 97.14%     | 97.84%          | 98.08%         | 98.44%         |
| AUS  | 86.20%       | 86.67%      | 86.20%     | 86.54%          | 87.46%         | 87.71%         |
| DIA  | 72.32%       | 72.96%      | 73.00%     | 72.19%          | 73.30%         | 73.30%         |
| GC   | 68.98%       | 71.00%      | 69.19%     | 68.74%          | 71.67%         | 69.90%         |
| SPL  | 81.41%       | 82.02%      | 81.78%     | 88.41%          | 89.86%         | 89.86%         |

To conclude the analysis, we wish to include some information on the CPU times needed to solve these problems. Table 5 reports the average solving time (in seconds) per fold of the models for the parameter values that provide the best AUC. For the approach in [Maldonado et al. (2018)](#), we report the time required by the two steps that are involved in the method.

Concerning the times of ex-OWA-SVM and ex-OWA-SVM$_K$, we note in passing that they correspond to formulation C-OWA-SVM$_K$ since, in all cases tested, the best results in terms of accuracy and AUC are obtained using monotone non-decreasing weights. Table 5 shows that the exact approach for OWA-SVM requires more time than the classical SVM and also more than the methods presented in [Maldonado et al. (2018)](#). This is due to the fact that models in [Maldonado et al. (2018)](#) have essentially the same complexity as the classical SVM.

The aforementioned results show that the exact OWA-SVM models introduced in this paper improve the classification performance metrics of the classical SVM. Furthermore, these measures are similar to the ones reported in previous approaches to OWA-SVM models in terms of ACC and AUC, although they have the advantage of actually capturing the essence of OWA in its application to SVM.
Table 5: Times per fold of each model for the best parameter values

| Data | \( \ell_2 \)-SVM | \( \ell_2 \)-SVM \(_K\) | ex-OWA-SVM | ex-OWA-SVM \(_K\) |
|------|-----------------|-----------------|------------|-----------------|
| IONO | 0.023           | 0.014           | 4.725      | 4.967           |
| WBC  | 0.003           | 0.003           | 0.006      | 0.003           |
| AUS  | 0.011           | 0.025           | 19.900     | 26.609          |
| DIA  | 0.013           | 0.009           | 25.133     | 21.536          |
| GC   | 0.033           | 0.016           | 41.788     | 31.707          |
| SPL  | 0.022           | 0.522           | 40.561     | 30.866          |

6 Conclusions

OWA operators have been applied to different problems of decision theory. This paper proposes an exact approach that allows the introduction of OWA operators for the deviation errors appearing in the soft-margin SVM. For this aim, we have distinguished between OWA-SVM with non-decreasing \( \lambda \)-weights and OWA-SVM with general \( \lambda \)-weights (not necessarily non-decreasing).

The use of non-decreasing weights allowed to formulate the model using only continuous variables. As consequence, a quadratic continuous formulation was developed, C-OWA-SVM. In addition, it was shown that non linear kernels could be accommodated in this model by the use of the dual formulation. The required solving time of this formulation is similar to the classical one. In contrast, the use of non-monotone weights in the OWA-SVM leads us to the use of binary variables to model the order of the deviations vector. Then, a mixed integer quadratic formulation, NC-OWA-SVM, is necessary to solve this problem. Hence, NC-OWA-SVM is more complex than C-OWA-SVM. Despite this, it is also possible to apply non-linear kernel by the use of an alternative formulation.

We have compared the proposed models with the heuristic approach to OWA-SVM appearing in Maldonado et al. (2018). Regarding the results, we can conclude that app-OWA-SVM provides solutions very different from the optimal solutions of the resulting model of applying actual OWA operators to SVM. However, both methodologies show similar predictive performance improving the ones obtained with the classical SVM (linear and non linear).

As future research, it could be interesting to analyze the OWA-SVM model using other \( \ell_p \)-norms. Besides, it could also be studied the integration of other aspects to OWA-SVM models such as feature selection, outlier detection or presence of label noise.
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