A novel embedded min-max approach for feature selection in nonlinear Support Vector Machine classification

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Abstract

In recent years, feature selection has become a challenging problem in several machine learning fields, particularly in classification problems. Support Vector Machine (SVM) is a well-known technique applied in (nonlinear) classification. Various methodologies have been proposed in the literature to select the most relevant features in SVM. Unfortunately, all of them either deal with the feature selection problem in the linear classification setting or propose ad-hoc approaches that are difficult to implement in practice. In contrast, we propose an embedded feature selection method based on a min-max optimization problem, where a trade-off between model complexity and classification accuracy is sought. By leveraging duality theory, we equivalently reformulate the min-max problem and solve it without further ado using off-the-shelf software for nonlinear optimization. The efficiency and usefulness of our approach are tested on several benchmark data sets in terms of accuracy, number of selected features and interpretability.

Keywords: Machine learning, min-max optimization, duality theory, feature selection, nonlinear Support Vector Machine classification

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1. Introduction

In the era of big data, where huge quantities of information are collected every day, the problem of determining which of these data are really important is a challenging task. Indeed, in recent years, the number of processes where hundreds or even thousands of features are collected has considerably increased. Here, a feature is defined as an individual and measurable property of the process. Thus, it is desirable to apply machine learning techniques to retrieve knowledge from data, or equivalently to know which are the most informative features, i.e., to perform feature selection. Hence, no wonder that feature selection algorithms are on trend, [5, 21].

The goal of feature selection is to remove the most irrelevant and redundant features to obtain an optimal feature subset. Feature selection has three main advantages: First, it enhances the interpretability of the results by building simpler models, [6, 28]. Second, it reduces the noise and leads to cleaner and more understandable data, [8, 11]. Finally, it may improve the prediction performance since overfitting is reduced, [7, 20].

A comprehensive description of different feature selection methods, including some examples and a brief discussion on their stability, is done in [12]. For the most recent surveys on this topic, the reader is referred to [22, 24].

Feature selection techniques can be applied in both regression, [4], and classification algorithms, [5, 32]. In this paper, we focus on feature selection methods for the well-known Support Vector Machine (SVM) binary classification problem, [13]. In plain words, SVM aims at finding the hyperplane that maximizes the minimum distance of the training points of different classes.

Feature selection techniques are usually classified into filter, wrapper and embedded methods, [12]. Filter methods act on the data without taking into account the machine learning technique that will be used to extract knowledge from them. Consequently, they are usually applied as a preprocessing step. They rank all the features according to a score function computed from the data and filter out the lowly ranked variables. While filter methods are com-
putationally fast and simple, they completely ignore the interaction with the learning approach.

Wrapper methods aim to find a subset of variables that gives the best predictor performance value. Two steps are performed in a wrapper method. First, a subset of features is selected, and second, the quality of such a subset is evaluated according to a score function based on the machine learning problem. This process is repeated until some stopping criterion is satisfied. Here, the learning machine acts as a black-box, but it somehow guides the final results. Nevertheless, since most of the computational time is spent on training the model, this type of feature selection method is rarely applied.

Finally, embedded methods simultaneously train the model and perform feature selection. That is, the learning part and the feature selection part are simultaneously performed. Therefore, they can be deemed as more “clever” methods than the filter strategies since they interact with the prediction model, and faster than the wrapper methods since the learning model does not need to be trained every time a feature subset is selected. The feature selection method for nonlinear SVM classification that we propose falls within this category.

Several works on the topic of embedded feature selection methods for SVM are currently available in the technical literature. In the linear setting, for instance, [30] proposes a model that is equivalent to solving the primal of the SVM problem with the $\ell_1$-norm, instead of the usual $\ell_2$-norm. The authors in [14] formulate an optimization problem that automatically tunes, via a bisection method, the number of features to be used, taking into account that this number cannot exceed a pre-fixed value. A mixed-integer linear program with a budget constraint that limits the number of features to be used is presented in [19]. Besides, two big-M-type constraints that link the continuous and binary variables are included. In order to guarantee tight enough values of such big Ms, the authors propose several strategies that imply the resolution of extra optimization problems before solving the feature selection program. To our knowledge, [18] was the first paper that performs an embedded feature selection method using a bilevel problem. The Karush-Kuhn-Tucker conditions are used to reformulate
it, and its relaxed version is solved with off-the-shelf nonlinear solvers. The authors of [2] extend the work in [18] by adding new binary variables in the upper-level problem to control the number of selected features.

Regarding embedded models for nonlinear SVM, most of them are based on regularization approaches, which trade-off between the SVM learning objective and the complexity of the resulting classification model. For example, [25, 35] penalize the objective function of the dual of the SVM problem with an approximation of the 0-“norm” of the feature vector. An ad-hoc strategy where six hyperparameters should be carefully tuned is proposed as the solving strategy. Four regularization-based approaches are formulated in [29]. DC (difference of convex functions) techniques are proposed to solve them. Another regularization strategy is given in [3], where a $\ell_1$-penalty term is added to the objective function. To solve such a problem, the kernel is linearized with respect to the feature weights to obtain a biconvex problem (in the classification and feature selection variables), which is then solved with gradient techniques in an alternating algorithm. The above-mentioned articles have proposed regularization methods with continuous variables. In contrast, a regularization model with binary variables, indicating if a feature is removed or not, is built in [33]. In particular, the authors of [33] perform feature selection by introducing binary variables in a model that minimizes a radius-margin bound on the leave-one-out error of the hard-margin SVM. The \{0, 1\}-variables are then relaxed to solve a penalized version of the proposed optimization problem via gradient-based approaches. In such a new model, the objective function now includes a penalization which controls, via a parameter conveniently tuned, the number of retained features. They also add a constraint which fixes the number of variables to be used. As for the approaches where binary variables are utilized to determine if a feature is removed or not, we should highlight the work of [26], where a mixed-integer nonlinear model with binary variables is built. The binary variables are iteratively updated according to a kernel-based classifier.

To sum up, the above-mentioned approaches can be classified into two groups. The first type of methodologies deal with the feature selection problem in linear
SVM, and therefore, they are unable to handle nonlinear separable data sets. The second group of references select the most relevant features in the nonlinear SVM classification at the expense of requiring ad-hoc solution algorithms with limited performance guarantees. To the best of our knowledge, none of the existing research works on this topic proposes a feature selection method for nonlinear SVM classification that can be seamlessly solved using off-the-shelf optimization software.

In this paper, we propose a novel embedded feature selection technique for nonlinear SVM classification that can be efficiently solved using off-the-shelf optimization software. Our technique involves solving a min-max optimization problem, where we balance two objectives, namely, the number of features to be used via the norm of their feature weights, and a proxy of the number of well-classified elements expressed in terms of the SVM margin. By way of duality theory, we reformulate this problem as a single-level equivalent problem that can be efficiently processed by off-the-shelf nonlinear solvers. This way, we avoid the use of arduous ad-hoc solution strategies that, besides, often rely on the tuning of multiple hyperparameters. The numerical experience performed in different data sets shows that our approach yields similar or even better results than alternative state-of-the-art methods, with the added distinct advantage of being simpler and easily implementable.

The remaining of this paper is structured as follows: Section 2 briefly introduces basic definitions and concepts regarding SVM. Section 3 formulates the proposed optimization problem, and explain how to solve it. Section 4 is devoted to the description of the data sets, experiments and comparative algorithms, and Section 5 details the numerical experience performed. We finish in Section 6 with some conclusions and possible extensions.

2. SVM Classification

We focus on the binary classification problem: Given two groups of labeled data, the aim is to predict the label of an unobserved point based on
the knowledge extracted from the training points. More precisely, consider a sample of individuals \( S \). For each individual \( i \in S \), we associate the pair \((x_i, y_i)\), where \( x_i \in \mathbb{R}^M \) is a \( M \)-dimensional vector representing the features, and \( y_i \in \{-1, +1\} \) denotes the label of the individual \( i \). The main goal is to find a classification rule to predict the label \( y \) of a new unseen individual using the information provided by \( x \).

Several strategies have been developed in the literature to handle the binary classification problem. See [17] for a review. In this paper, we apply the well-known and extensively used method known as Support Vector Machine (SVM), [13]. The primal formulation of the soft-margin SVM problem is as follows:

\[
\begin{align*}
\min_{w, b, \xi} & \frac{1}{2} \|w\|^2 + C \sum_{i \in S} \xi_i \\
\text{s.t.} & \quad y_i (w' x_i + b) \geq 1 - \xi_i, \forall i \\
& \quad \xi_i \geq 0, \forall i
\end{align*}
\]

(1a) (1b) (1c)

where the best separating hyperplane has the form \( w' x + b = 0 \). The normal vector to the hyperplane is denoted by \( w \in \mathbb{R}^M \), \( b \) indicates a threshold value, and the prime denotes the transpose, e.g., \( w' \). In addition, the notation \( r' s \) indicates the dot product between the vectors \( r \) and \( s \), i.e., \( r' s = \sum r_i s_i \). Finally, a regularization parameter \( C \) is introduced to penalize the misclassified points via the slack variables \( \xi_i, \forall i \).

The following linear classification rule is derived from the optimal solution of Problem (1): A new unseen point \( x \) is classified in class 1 if and only if \( \hat{y}(x) + b \geq 0 \), where \( \hat{y}(x) \) is the so-called score function, defined as:

\[
\hat{y}(x) = w' x
\]

(2)

SVM cannot only handle linear binary classification problems but is also able to deal with nonlinear separable training points by means of the kernel trick. The key idea is to translate the original data \( x_i \) to a higher dimensional space \( \mathcal{X} \) through a feature map \( \phi : \mathbb{R}^M \to \mathcal{X} \), where the data become linear. Hence,
Problem (1) can be written in terms of the transformed data, \( \phi(x_i) \) as follows:

\[
\begin{align*}
\min_{w, b, \xi} & \quad \frac{1}{2} \|w\|^2 + C \sum_{i \in S} \xi_i \\
\text{s.t.} & \quad y_i (w' \phi(x_i) + b) \geq 1 - \xi_i, \forall i \\
& \quad \xi_i \geq 0, \forall i
\end{align*}
\]

(3a) (3b) (3c)

The score function \( \tilde{y} \) is, therefore, modified as indicated below:

\[ \tilde{y}(x) = w' \phi(x) \]  

(4)

It is quite obvious that the nonlinear case can be reduced to the linear one, just setting \( \phi(x) = x \). Unfortunately, the expression of \( \phi \) is usually unknown and consequently, Problem (3) cannot be solved in practice. However, this issue is handled by resorting to the dual formulation of (3):

\[
\begin{align*}
\max_{\alpha} & \quad \sum_{i \in S} \alpha_i - \frac{1}{2} \sum_{i, \ell} \alpha_i \alpha_{\ell} y_i y_{\ell} \phi(x_i)' \phi(x_{\ell}) \\
\text{s.t.} & \quad \sum_{i \in S} \alpha_i y_i = 0, \\
& \quad 0 \leq \alpha_i \leq C, \forall i
\end{align*}
\]

(5a) (5b) (5c)

Problem (5) maximizes a quadratic concave objective function with linear constraints. Hence, it can be solved with standard convex optimization solvers. Moreover, as a consequence of the Lagrange dual reformulation of Problem (3), it holds that the coefficients of the hyperplane normal vector, \( w \), can be expressed in terms of the \( \alpha \) variables, as follows:

\[ w = \sum_{i \in S} \alpha_i y_i \phi(x_i) \]  

(6)

and, therefore, the score function \( \tilde{y}(x) \) in (4) turns out to be:

\[ \tilde{y}(x) = \sum_{i \in S} \alpha_i y_i \phi(x_i)' \phi(x) \]  

(7)

Note that both the resolution of Problem (5) and the evaluation of the score function in (7) do not depend on computing the value of \( \phi \) (whose explicit
form is unknown), but on computing the value of the dot product \( \phi(x_i)' \phi(x_\ell) \), \( \forall (i, \ell) \). This tremendously simplify the calculation of a nonlinear classification rule by way of SVM. Indeed, it suffices to select a so-called kernel function, \( K : \mathbb{R}^M \times \mathbb{R}^M \to \mathbb{R} \), as such a dot product, i.e.:

\[
K(x_i, x_\ell) = \phi(x_i)' \phi(x_\ell), \quad \forall i, \ell
\]  

Consequently, the score function (7) can be written as:

\[
g(x) = \sum_{i \in S} \alpha_i y_i K(x_i, x_\ell) \quad (9)
\]

and Problem (5) can be recast as:

\[
\begin{cases}
\max \alpha \sum_{i \in S} \alpha_i - \frac{1}{2} \sum_{i, \ell} \alpha_i \alpha_\ell y_i y_\ell K(x_i, x_\ell) \\
\text{s.t.} \sum_{i \in S} \alpha_i y_i = 0, \forall i \\
0 \leq \alpha_i \leq C, \forall i
\end{cases}
\]  

(10a) (10b) (10c)

Intuitively, the kernel function implicitly gives us access to a (possibly infinite dimensional) family of feature mappings \( \phi(\cdot) \) without actually having to work with them. In the next section, we elaborate on how we propose to enrich problem (10) with the ability to automatically perform feature selection.

3. Feature Selection Methodology

This section details the proposed approach to select the most relevant features when classifying. Particularly, in Section 3.1, we formulate a min-max optimization program to solve the feature selection problem. Section 3.2 explains how to reformulate such a problem to be then solved with off-the-shelf software in Section 3.3.

3.1. Min-max problem formulation for feature selection

The kernel trick in the dual formulation (10) reveals that, for linearly separating the data in a certain feature space \( \mathcal{X} \), it is not necessary to know the
explicit expression of the mapping $\phi(\cdot)$, but of the associated dot product or
kernel $K(x_i, x_\ell) = \phi(x_i)'\phi(x_\ell)$, $\forall i, \ell$. Actually, it can be considered that all
the maps $\phi(\cdot)$ reproduced by the same kernel are equivalent, [27]. No wonder,
therefore, that the success of the nonlinear SVM problem highly relies on a care-
ful selection of the kernel. In this vein, our approach aims to identify a kernel
whereby the SVM is able to separate the data (as much as possible) using the
most informative features only.

Following this argument, consider next a family of kernels $K_\gamma(\cdot, \cdot)$ parameterized in terms of a finite-dimensional vector $\gamma$. Each member in this family reproduces a catalog of feature maps $\phi(\cdot)$ in a feature space $F_\gamma$. We can now re-
formulate the primal version of the nonlinear SVM to account for this additional
degree of freedom as follows:

$$
\begin{align}
\min_{\gamma} \min_{w, b, \xi} & \frac{1}{2} \|w\|^2 + C \sum_{i \in S} \xi_i \\
\text{s.t.} & \quad y_i (w' \phi(x_i) + b) \geq 1 - \xi_i, \forall i \\
& \quad \xi_i \geq 0, \forall i, \\
& \quad \phi \in F_\gamma,
\end{align}
$$

where we also look for the best $\gamma$, i.e., the best functional space $F_\gamma$, that maxi-
mizes the SVM soft margin.

Unsurprisingly, problem (11) is intractable, now not only because the par-
ticular form of the feature map $\phi(\cdot)$ is unknown, but also because we do not
have an explicit expression of the feature space $F_\gamma$ in terms of the parameter
vector $\gamma$. In a first step to cope with this challenge, we resort again to the dual
formulation of the nonlinear SVM, that is:

$$
\begin{align}
\min_{\gamma} \max_{\alpha} & \sum_{i \in S} a_i - \frac{1}{2} \sum_{i, \ell} a_i a_\ell y_i y_\ell K_\gamma(x_i, x_\ell) \\
\text{s.t.} & \quad \sum_{i \in S} a_i y_i = 0, \forall i \\
& \quad 0 \leq a_i \leq C, \forall i
\end{align}
$$

As opposed to (11), the good thing about problem (12) is that we may indeed
have an explicit expression of a kernel \( K_\gamma(\cdot, \cdot) \) in terms of a finite-dimensional parameter vector \( \gamma \). For instance, in this paper, we will work with the anisotropic Gaussian kernel with bandwidth parameter \( \gamma \geq 0 \), which is well known for its flexibility and which takes the following form:

\[
K_\gamma(x_i, x_\ell) = \exp \left( - \sum_{j=1}^{M} \gamma_j (x_{ij} - x_{\ell j})^2 \right) \quad (13)
\]

In particular, the anisotropic Gaussian kernel will allow us to perform feature selection via feature weighting in a natural way. In effect, using the expression in (13), the importance of each feature can be easily measured through the value of \( \gamma_j \). More precisely, values of \( \gamma_j \) tending to zero imply that the associated feature \( j \) plays no role in the classification. In contrast, larger values of \( \gamma_j \) indicate that feature \( j \) is critical for obtaining good classification results.

A major drawback of problem (12) (or equivalently, of problem (11)) is, however, that the additional degree of freedom introduced by the parameter vector \( \gamma \) is likely to produce overfitting of the training data. Indeed, it is known that values of \( \gamma_j \) tending to infinite in the Gaussian kernel (13) will lead to this troublesome phenomenon. Consequently, we somehow need to penalize large values of \( \gamma \) in problem (12). At the same time, if \( \gamma_j = 0, \forall j \), then the kernel expression (13) is equal to one for all pair of individuals in the sample, i.e., \( K_\gamma(x_i, x_\ell) = 1, \forall i, \ell \). It is thus easy to check by combining the SVM classification rule (2), the score function (9) and constraint (12b) that the predicted label of a new unseen individual, in this case, will always coincide with the sign of \( b \), resulting in poor classification performance.

Hence, it is quite apparent that there exists a trade-off between model complexity and classification accuracy. In other words, a model that simultaneously minimizes the feature weights and maximizes the accuracy is desired. To this aim, we modify Problem (12) to propose the min-max optimization problem (14), where a trade-off between two objectives, namely the \( p \)-(pseudo)norm of the feature weights vector \( \gamma \), \( \|\gamma\|_p \), for \( p \geq 0 \), and the objective function of the SVM problem (10) is to be optimized. The importance associated with each
objective is measured in terms of parameter $C_2$, which balances the complexity of the model and the classification accuracy and whose value depends on the user’s preferences. Values of $C_2$ close to 0 favor models with high in-sample prediction accuracy even though the number of features to be used is large. Conversely, $C_2$ values tending to 1 result in models with a reduced number of features at the expense of sacrificing some accuracy.

$$\min_{\gamma \geq 0} \left[ C_2 \|\gamma\|_p^p + (1 - C_2) \max_{\alpha} \frac{1}{2} \sum_{i \in S} \alpha_i - \frac{1}{2} \sum_{i, \ell \in S} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell) \right] \quad (14a)$$

subject to:

$$\sum_{i \in S} \alpha_i y_i = 0 \quad (14b)$$

$$0 \leq \alpha_i \leq C, \forall i \quad (14c)$$

Compared to the rest of embedded approaches for nonlinear SVM classification in the technical literature, our model (14) does not select the most relevant features via binary variables, as in [26, 33]. In contrast, we perform feature selection through feature weighting by means of continuous variables. This way, we do not only avoid the difficulties associated to Integer Programming, but we also get to know whether a feature is relevant or not, together with some measure of its degree of importance.

Furthermore, all the models proposed in [3, 25, 29] penalizes the size of the feature vector within the objective function of the dual SVM problem (10). However, our goal is to find the $\gamma$ that leads to the largest SVM margin. This implies minimizing over $\gamma$ the minimum of $\frac{1}{2} \|w\|^2 + C \sum_{i \in S} \xi_i$ over $w$ and $\xi$, as in (11), or equivalently, minimizing over $\gamma$ the maximum of $\sum_{i \in S} \alpha_i - \frac{1}{2} \sum_{i, \ell} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell)$ over $\alpha$, as in (12). Since we still want to leverage the kernel trick, we need to opt for the latter and introduce the regularization term accordingly as in (14). This gives rise to the min-max approach for feature selection that we propose.

3.2. Model Reformulation

Problem (14) is a nonconvex optimization problem very hard to solve, in general. The aim of this section is to reformulate such a problem in order to solve it via off-the-shelf software.
First of all, we equivalently rewrite Problem (14) using its epigraph form as:

\[
\begin{align*}
\min_{\gamma \geq 0, z} & \quad C_2 \|\gamma\|_p^p + (1 - C_2)z \\
\text{s.t.} & \quad z \geq \max_{\alpha} \alpha_i - \frac{1}{2} \sum_{i,\ell \in S} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell) \\
& \quad \sum_{i \in S} \alpha_i y_i = 0 \\
& \quad 0 \leq \alpha_i \leq C, \forall i
\end{align*}
\] (15a)

Problem (15) can be seen as a bilevel optimization problem where the upper-level problem aims at obtaining good classification results with a low number of features, whereas the lower-level problem focuses on the classification task. Indeed, the lower-level problem states that the decision variable \(z\) is lower-bounded by the optimal solution of the dual SVM problem (10).

In order to solve Problem (15), we propose a reformulation based on the lower-level dual problem, which exploits the fact that the SVM problem (10) is a convex optimization problem with a quadratic objective function and affine constraints. Hence, strong duality holds and the lower-level problem (15b) - (15d) can be equivalently replaced by its dual, (10). Actually, strong duality also allows us to justify the outer minimization in (14) using arguments from Mathematical Programming: Maximizing the SVM soft margin involves minimizing objective function (11a), which, in turn, takes on the same value as that of the dual objective (12a) at the primal and dual optima. Therefore, we are to minimize the dual objective (12a) over \(\gamma\).

We start then building the Lagrangian function of the lower-level problem. For the sake of simplicity, in what follows, matrix notation will be used. We define \(G_\gamma := diag(y)K_\gamma diag(y)\) as the quadratic form of the SVM problem, and \(diag(y)\) represents the matrix with the vector \(y\) in its diagonal. Moreover, \(e\) represents a vector full of ones of appropriate dimension, and the variables between brackets next to the constraints (15c) and (15d) are their corresponding dual decision variables. With this notation, the Lagrangian function of the lower-
level problem is computed as follows:

\[ L(\alpha, \nu, \lambda_0, \lambda^C) = e'\alpha - \frac{1}{2} \alpha'G\gamma\alpha - \nu y'\alpha + (\lambda^0)'\alpha - (\lambda^C)'(\alpha - Ce) \]  \hfill (16)

To compute the objective function of the dual of the lower-level problem, it is necessary to compute the gradient of \( L(\alpha, \nu, \lambda_0, \lambda^C) \) with respect to \( \alpha \),

\[ \nabla_\alpha L(\alpha, \nu, \lambda_0, \lambda^C) = e - G\gamma\alpha - \nu y + \lambda_0^0 - \lambda^C \]  \hfill (17)

Therefore, the dual formulation of the SVM problem \[10\] is:

\[
\begin{cases}
\min_{\alpha, \nu, \lambda_0, \lambda^C} -\frac{1}{2} \alpha'G\gamma\alpha + (e - \nu y + \lambda_0^0 - \lambda^C)'\alpha + C(\lambda^C)'e \\
\text{s.t. } G\gamma\alpha - (e - \nu y + \lambda_0^0 - \lambda^C) = 0 \\
\lambda_0^0, \lambda^C \geq 0
\end{cases}
\] \hfill (18a)

and Problem \[15\] is equivalent to:

\[
\begin{cases}
\min_{\gamma,z} C_2\|\gamma\|_p^p + (1 - C_2)z \\
\text{s.t. } z \geq \min_{\alpha, \nu, \lambda_0, \lambda^C} -\frac{1}{2} \alpha'G\gamma\alpha + (e - \nu y + \lambda_0^0 - \lambda^C)'\alpha + C(\lambda^C)'e \\
\text{s.t. } G\gamma\alpha - (e - \nu y + \lambda_0^0 - \lambda^C) = 0 \\
\gamma, \lambda_0^0, \lambda^C \geq 0
\end{cases}
\] \hfill (19a)

The second term of the objective function \[19a\] aims at minimizing \( z \), which is a variable lower-bounded by the optimal objective value of Problem \[18\]. Hence, the optimal decision variable \( z \) can be replaced by the optimal value of Problem \[18\], and Problem \[19\] is written as:

\[
\begin{cases}
\min_{\gamma, \alpha, \nu, \lambda_0, \lambda^C} C_2\|\gamma\|_p^p - (1 - C_2) \left( \frac{1}{2} \alpha'G\gamma\alpha - (e - \nu y + \lambda_0^0 - \lambda^C)'\alpha - C(\lambda^C)'e \right) \\
\text{s.t. } G\gamma\alpha - (e - \nu y + \lambda_0^0 - \lambda^C) = 0 \\
\gamma, \lambda_0^0, \lambda^C \geq 0 \\
0 \leq \alpha \leq C
\end{cases}
\] \hfill (20a)

Problem \[20a\]-\[20d\] is the single-level equivalent reformulation of the bilevel optimization problem \[15\]. It is strongly non-convex and, as a result, we can
only aspire to get local optimal solutions if nonlinear optimization solvers are used. In this regard, our numerical experiments reveal that including constraints \((20d)\), albeit redundant, helps the nonlinear solver to reach a good local optimal solution faster, especially for large values of \(C_2\). In Section 3.3, we elaborate on a simple but effective solving strategy based on off-the-shelf optimization software.

3.3. Solving Strategy

The aim of this section is to detail the strategy carried out to solve Problem \((20)\). We propose a generic efficient method based on grid search approaches and standard off-the-shelf solvers.

Firstly, we must clarify that, in order to avoid overfitting and to obtain stable results, the whole sample of individuals \(S\) is divided into a training and test subsamples denoted by \(\tilde{S}\) and \(S_{\text{test}}\), respectively. This process is repeated \(k\) times so that there is no common individual between the test samples of two different iterations. Secondly, the proposed feature selection approach is solved for a fixed value of the hyperparameter \(C_2\) defined by the user.

The first step when solving Problem \((20)\) is to determine the value of hyperparameter \(C\) and to find an appropriate starting point of the \(\gamma\) variable vector, \(\gamma^{\text{ini}}\), for the nonlinear off-the-shelf solver. In this paper, we opt to choose the best \(\gamma\) provided by the standard SVM problem \((10)\), where no feature selection is performed, i.e., for the \(\gamma\) value which gives the best predictions, when assuming that all the features play the same role and, consequently, setting \(\gamma_j = \gamma, \forall j\) in the kernel function \((13)\). To this aim, \(N\)-fold cross-validation has been implemented. At each iteration, sample \(\tilde{S}\) is divided into training and validation data, denoted respectively as \(S_{\text{tr}}\) and \(S_{\text{val}}\). Hence, for a fixed \((C, \gamma)\) varying in a grid previously selected, Problem \((10)\) is solved in \(S_{\text{tr}}\) with \(\gamma_j = \gamma, \forall j\). For fixed values of \(\gamma\), optimization problem \((10)\) is convex and can be solved using commercial optimization software. The selected pair \((C^* , \gamma^{\text{ini}})\) is chosen to be the one that maximizes the averaged accuracy on \(S_{\text{val}}\) over the \(N\) folds.

Once the optimal value of \(C\) and the initial solution \(\gamma^{\text{ini}}\) are determined,
the dual formulation of the lower-level problem \(18\) is solved in \(\tilde{S}\) to obtain the initial decision variables \(\alpha^{ini}\), \(\nu^{ini}\), \(\lambda^{0,ini}\), and \(\lambda^{C,ini}\). For fixed \(C\) and \(\gamma\), this problem is also convex and can be solved with commercial optimization software.

Next, we solve Problem \(20\) in sample \(\tilde{S}\) for the same value \(C^*\) and using the initial decision variables as a starting point. To do this, we use an off-the-shelf nonlinear solver. To guarantee that we work with \(\alpha\) decision variables that are globally optimal for the so obtained \(\gamma_j\) for all feature \(j\), we then solve the convex Problem \(10\) in \(\tilde{S}\) for such a \(\gamma\) vector.

Finally, the efficiency of our approach is measured by computing the accuracy on sample \(S_{test}\) using the corresponding decision variables, \(\alpha\) and \(\gamma\), previously determined, by solving Problems \(10\) and \(20\), respectively.

A pseudocode of our solving strategy for a certain division of sample \(S\) is sketched in Algorithm \([\text{4}]\).

In summary, the proposed solution strategy requires solving \(N\) convex optimization problems, for each pair \((C, \gamma)\), one convex optimization problem for fixed \(C^*\), and one nonconvex optimization problem. Laborious and complex ad-hoc methodologies are not necessary here.

4. Experimental Setup

All the computational experiments carried out in this research are detailed in this section. Section 4.1 is devoted to the description of the data sets employed in our analyses. Section 4.2 explains the experiments performed. Finally, Section 4.3 introduces the algorithms our approach is compared with.

4.1. Data Sets

We have worked with four databases, namely breast, diabetes, lymphoma, and colorectal, all of which can be downloaded from [31]. Table 1 includes the number of individuals, the number of features, and the percentage of individuals of the predominant class in each of these databases.
Algorithm 1 Solving strategy for the proposed min-max approach

**Input:** sample division $\tilde{S}$ and $S_{test}$, and hyperparameter $C_2$.

**Computation of initial solution**

for fold in $1,\ldots,N$ do

• Define samples $S_{tr}$ and $S_{val}$.

for $(C, \gamma)$ in the grid do

• Solve SVM problem (10) on $S_{tr}$ with $\gamma_j = \gamma, \forall j$ in kernel (13).

• Compute accuracy on $S_{val}$.

end for

end for

• $(C^*, \gamma^{ini}) = \arg\max_{(C, \gamma)} \text{averaged accuracy}_{S_{val}}(C, \gamma)$

• Solve Problem (18) in $\tilde{S}$ for $C^*$ and starting at $\gamma^{ini}$. Obtain $\alpha^{ini}$, $\nu^{ini}$, $\lambda_0^{ini}$, and $\lambda^{C,ini}$.

**Computation of local optimal solution**

• Solve Problem (20) on $\tilde{S}$ for $C^*$ and starting at $(\gamma^{ini}, \alpha^{ini}, \nu^{ini}, \lambda_0^{ini}, \lambda^{C,ini})$.

**Computation of global optimal solution $\alpha$**

• Solve Problem (10) in $\tilde{S}$ for fixed $\gamma$ obtained from the previous step.

**Output:** Optimal hyperparameter $C^*$, optimal decision variables $\gamma$, $\alpha$, $\nu$, $\lambda^0$ and $\lambda^C$, and the classification accuracy on $S_{test}$.

| Data set   | # individuals | # features | % predominant class |
|------------|---------------|-----------|---------------------|
| breast     | 569           | 30        | 63%                 |
| diabetes   | 768           | 8         | 65%                 |
| lymphoma   | 96            | 4026      | 64%                 |
| colorectal | 62            | 2000      | 65%                 |

Table 1: Data description summary

*Diabetes* is likely a nonlinearly separable data set, as [1] affirms and our numerical experiments below reveal.

*Colorectal* is known to contain outliers, [9]. Indeed, improvements in classification accuracy of up to 8-9 percentage points have been reported if those outliers are removed. A discussion on the impact of the outliers on our approach in comparison with other strategies is detailed in Section 5. To this end, we have
considered as outliers the 11 individuals (out of 62) identified in [16].

4.2. Description of the Experiments

This section elaborates on the experiments carried out to assess and benchmark our approach, which will be denoted in Section 5 as MM-FS.

As a preprocessing step, the features of each data set have been normalized so that each feature belongs to the interval $[-1, 1]$. Algorithm 1 has been run to show the efficiency and usefulness of the proposed methodology. Indeed, in order to get stable results, the experiment given in Algorithm 1 has been performed $k = 10$ times. More specifically, the whole sample $S$ has been divided into 10 folds. At each iteration, 1 out of the 10 folds is used as the test sample $S_{test}$. The remaining 9 folds form the $\tilde{S}$ sample. Note that there is no common individual between the test samples of two different iterations.

When computing the initial solution in Algorithm 1 the 9 folds are further subdivided into $N = 5$ folds, so that $S_{tr}$ and $S_{val}$ comprise, respectively, $\frac{4}{5}$ and $\frac{1}{5}$ of the data in such 9 folds. Problem (10) is solved on $S_{tr}$ as indicated in Algorithm 1. This process is repeated following a 5-fold cross-validation process.

The $\gamma$ grid of the initial solution is $\{10^{-4}, \ldots, 10^4\}$ and the hyperparameter $C$ moves in the set $\{10^{-4}, \ldots, 10^{-1}, 1, 2, \ldots, 9, 10, \ldots, 10^4\}$. The $p$ value chosen in the first term of the objective function (20a) is $p = 1$.

As explained in Section 3.1 here we assume that the hyperparameter $C_2$ should be chosen by the user. Hence, in this paper, we do not provide the results of our approach for a single value of $C_2$, but a curve of the out-of-sample accuracy versus the number of features retained for different values of $C_2$ in a range. If a value of $C_2$ were to be chosen based on a specific user’s criterion, then it would be selected, as usually done in the literature, according to the best results obtained in a validation sample in terms of that particular criterion.

Moreover, we show that our approach is able to achieve models with a low number of features even though a bit of accuracy is lost. To this aim, for a fixed $C_2$, we provide a curve where the success rate in the percentage of out-of-sample predictions is estimated in terms of the number of features selected.
To build this curve, we proceed as follows. Suppose we want to retain the \( F \) most informative features only in the SVM classification model. For this, we do a list in which each feature \( j \) is ranked according to the \( j \)-th component, \( \gamma_j \), of \( \gamma \) given by Algorithm 1. Then, we take the \( F \) most important features in the rank with their respective \( \gamma_j \) and solve Problem 10 in sample \( \tilde{S} \) with \( \gamma_j = 0 \) for all the non-selected features. This process is executed per fold, in such a way that we compute the percentage of those individuals in \( S_{test} \) that our approach correctly classifies over all folds. Finally, this percentage together with the value \( F \) yields a point in the curve.

Besides, in order to test the ability of our approach to producing interpretable SVM classification models, we also provide the name of those features which our method identifies as the most important ones and compare them with the features that are deemed as the most meaningful in the technical literature.

To sum up, our experiments provide: i) the efficient frontier “out-of-sample classification accuracy vs. norm of features weights” that our approach is able to deliver by varying \( C_2 \) in the grid \{0.01, 0.1, 0.2, \ldots, 0.8, 0.9, 0.99\}; ii) the percentage classification accuracy of our approach as features are gradually accounted for in order of importance, and iii) a discussion on the level of interpretability of the selected features.

All the experiments are carried out on a cluster with 21 Tb of RAM memory, running Suse Leap 42 Linux distribution. Models are coded in Python 3.7 and Pyomo 5.2 and solved using Cplex 12.6.3 for the convex problems and Ipopt 3.12.8 for nonconvex problems within a time limit of 24 hours.

4.3. Comparative Algorithms

Three alternative approaches have been used to compare our proposal. The first one, denoted as NO-FS, corresponds to the solution provided when no feature selection is made, i.e. when the importance of the features is given by a unique value \( \gamma_j = \gamma, \forall j \) in (13). In other words, the NO-FS method boils down to the classification results given by the initial solution of Algorithm 1.

The second approach, named KP-FS, is proposed in [25]. This model is
based on a regularization of the dual SVM problem, where an approximation of
the 0-“norm” is added as a penalty term in the objective function. This problem
is solved using a heuristic alternating algorithm that requires the careful tuning
of several hyperparameters.

The results provided by $KP-FS$ are based on ad-hoc solution strategies. For
this reason, the feature selection approach given by reference $[25]$ is denoted
as $KP-FS$ ad-hoc. Moreover, for the sake of comparison, we have also run the
feature selection model $KP-FS$ using off-the-shelf solvers. This comparative
strategy is named $KP-FS$ off-the-shelf. The values of some setting parameters
used in the $KP-FS$ off-the-shelf methodology should be defined. For instance,
the $\beta$ parameter which appears in the 0-“norm” approximation is set to five as
the authors suggested. Both steps of the alternating approach have been solved
with off-the-shelf software. In fact, the convex optimization problem of the
first step is solved using Cplex 12.6.3, whereas Ipopt 3.12.8 has been run
to solve the nonlinear optimization problem of the second step. The maximum
number of iterations of the alternating approach is set to five. In order to
avoid getting stuck at local optima, a multistart with three runs is performed
in the second step. The regularization parameter $C$ takes values in the set
$\{10^{-4}, \ldots, 10^{-1}, 1, 2, \ldots, 9, 10, \ldots, 10^4\}$ and the hyperparameter $C_2$
ranges in the set $\{0.01, 0.1, 0.2, \ldots, 0.8, 0.9, 0.99\}$.

The third approach, denoted by $MILP-FS$, has been proposed in $[19]$. The
authors of $[19]$ tackle the feature selection problem in linear SVM using a Mixed
Integer Linear Problem (MILP), where the maximum number of selected fea-
tures is chosen in advance. They devised two strategies to solve the resulting
MILP, namely, a heuristic approach and an exact procedure. In both cases,
extra optimization problems are to be solved.

As occurred in the $KP-FS$ approach, the solving strategy proposed in the
$MILP-FS$ method is based on ad-hoc procedures. For this reason, this method
will be denoted as $MILP-FS$ ad-hoc. We also propose to solve the $MILP-FS$
model using off-the-shelf optimization solvers. This comparative algorithm is
named as $MILP-FS$ off-the-shelf. In this approach, the SVM parameter $C$ also
moves in the set \( \{10^{-4}, \ldots, 10^{-1}, 1, 2, \ldots, 9, 10, \ldots, 10^4\} \), even though our experiments show that the \( C \) parameter seems not to play an important role when solving the MILP model. The budget parameter \( B \), which controls the maximum number of features to be selected is set to 10, 50, 5, and 50 for the databases breast, colorectal, diabetes and lymphoma, in that order. The lower and upper bounds used for the big-M constraints are fixed to \(-1\) and \(1\) in the data sets colorectal, diabetes and lymphoma, and \(-200\) and \(200\) in the database breast. This MILP model is solved using Cplex 12.6.3 with the default options.

The division of the whole data set into samples \( \tilde{S} \) and \( S_{\text{test}} \) used in KP-FS off-the-shelf and MILP-FS off-the-shelf has been performed in the very same manner as done for our MM-FS approach. Unfortunately, we do not know the exact sample division that was used for the KP-FS ad-hoc and MILP-FS ad-hoc approaches in [25] and [19], respectively. Thus, the results provided in Section 5 for these strategies are a verbatim transcript of those given in [25] and [19].

5. Numerical Experience

Next, we elaborate on the results delivered by the numerical experiments we have conducted. More precisely, in Section 5.1 we compare the results obtained with our method in terms of classification accuracy with respect to the other algorithms previously described. Section 5.2 discusses prediction results when just the most important features are used in the classification, and finally, Section 5.3 focuses on the interpretability of the selected features.

5.1. Accuracy results

As it was stated in Section 4.2 we do not provide the output results for a single value of \( C_2 \), but for all the values of \( C_2 \) in a prefixed grid. In particular, Figure 1 shows a curve for all the databases where the norm of the weights \( \gamma \) versus the percentage of well classified over the 10 folds is represented. Unsurprisingly, in the four data sets, we can see that the larger the value of \( C_2 \), the lower the norm of the weights \( \gamma \). On the other hand, the averaged test accuracy does not feature such a smooth behavior in terms of the \( C_2 \) values as the
The $\gamma$-norm does. This is due to two reasons. First, because the second term of the objective function (20a) does not maximize the accuracy, but a proxy of it given by the SVM margin. Second, the performance of model (20) is optimized over the sample data $\tilde{S}$, which provide an incomplete view of reality. Consequently, this performance may not necessarily generalize to the test set, $S_{test}$.

The main take-away of these figures is that values of $C_2$ very close to 0 or 1 lead to low accuracy levels in the test set. Low values of $C_2$ yield complex models that tend to overfit the data and reduce out-of-sample performance. This is especially noticeable in data sets colorectal and lymphoma, where the ratio between the number of features and the number of individuals is larger. Conversely, high values of $C_2$ produce oversimplified models unable to capture all the explanatory power of the available features.

Figure 1: Plot of the percentage of well-classified on sample $S_{test}$ over 10 folds versus the 1-norm of weights $\gamma$. 
Table 2 shows the best accuracy results in the test sample with our approach together with the $C_2$ value at which such accuracy is reached. We also include the accuracy results obtained in the test samples for all the comparative algorithms presented in Section 4.3. We recall that the sample division used in methodologies NO-FS, KP-FS off-the-shelf and MILP-FS off-the-shelf is exactly the same as that considered in our MM-FS approach. Moreover, the accuracy of the methods KP-FS ad-hoc and MILP-FS ad-hoc has been directly taken from [25] and [19], respectively. In this vein, the lymphoma data set has not been used in MILP-FS ad-hoc, and therefore, its accuracy result is not available. In addition, databases colorectal and lymphoma cannot be solved by the KP-FS off-the-shelf approach within a time limit of 24 hours.

|                  | breast | diabetes | lymphoma | colorectal |
|------------------|--------|----------|----------|------------|
| MM-FS            | 97.35% | 76.43%   | 96.87%   | 85.48%     |
| $C_2$ accuracy MM| 0.7    | 0.3      | 0.1      | 0.9        |
| NO-FS            | 97.89% | 77.08%   | 94.79%   | 83.87%     |
| KP-FS ad-hoc     | 97.55% | 76.74%   | 99.73%   | 96.57%     |
| KP-FS off-the-shelf| 62.74% | 65.10%   | Max time | Max time   |
| MILP-FS ad-hoc   | 97.72% | 77.75%   | Not avail.| 92.08%     |
| MILP-FS off-the-shelf | 96.48% | 67.44%   | 97.91%   | 85.48%     |

Table 2: Accuracy results for our MM-FS approach and all the comparative algorithms.

We observe that the proposed MM-FS approach obtains similar accuracy results than those achieved with the NO-FS method, where all the features have the same weights. In other words, our approach is able to successfully extract the relevant information of the data by selecting the features with the highest classification power. Interestingly, in some cases, such as for the databases colorectal and lymphoma, the elimination of irrelevant features by our approach improves the prediction accuracy.

Remarkably, our approach, which makes use of available off-the-shelf optimization software, delivers results that are comparable to those given by the ad-hoc implementations of KP-FS and MILP-FS for all databases, except for colorectal, which will be later discussed.
With respect to the comparative algorithm *KP-FS off-the-shelf*, the results reveal that our *MM-FS* approach is significantly better in databases *breast* and *diabetes*. In particular, when the *KP-FS* model is solved with off-the-shelf software, it turns out that the $\gamma$ variables of all features tend to zero, leading to inaccurate predictions, where all the elements are classified with the label of the predominant class. In the case of *lymphoma*, it is even impossible to obtain a local optimal solution within the time limit of 24 hours. The results obtained with the *MILP-FS off-the-shelf* are slightly better than those of the *MM-FS* methodology for the *lymphoma* data set. In contrast, our proposal is slightly better than *MILP-FS off-the-shelf* for the *breast*. Finally, it can be seen that our *MM-FS* approach delivers significantly better results than *MILP-FS off-the-shelf* for the *diabetes* data set. In fact, the *MILP-FS off-the-shelf* just predicts correctly the predominant class. This is most likely due to the fact that *MILP-FS off-the-shelf* is limited to linear classifiers, while the *diabetes* data set is, however, not linearly separable, as indicated in Section 4.1.

We conjecture that the differences observed for data set *colorectal* when comparing our *MM-FS* strategy with algorithms *KP-FS ad-hoc* and *MILP-FS ad-hoc* are due to the significant number of outliers that this data set, of only 62 individuals, contains. Unfortunately, there is no comment on the treatment of outliers in [25] or [19]. However, our conjecture is based on the following two facts: i) if these outliers are removed from the data set, the performance of our approach is comparable to that reported for *KP-FS ad-hoc* and *MILP-FS ad-hoc* in [25] and [19], respectively; and ii) the estimated accuracy of the *off-the-shelf* variant of *MILP-FS* is the same as that of our method.

Finally, we do not report an estimated accuracy value for method *KP-FS off-the-shelf*, since it provides no solution within the 24-hour limit.

5.2. Feature selection results

In this section, we assess the ability of our approach to select the most relevant features in a data set without impairing, as much as possible, the classification accuracy. For this purpose, next, we show results from a series
of experiments in which we analyze the performance of a nonlinear SVM that considers only the most relevant features identified by our method with their respective $\gamma$ values. Accordingly, the $\gamma$ values of the non-selected features are set to zero, as explained in Section 4.2.

![Figure 2: Plots of the percentage of well-classified estimated on sample $S_{test}$ over 10 folds for different number of ranked features of the MM-FS approach.](image)

Figure 2 shows the classification accuracy of the proposed approach over the 10 test sets (one per fold) for a different number of ranked features. Each subfigure pertains to one database. These results correspond to the $C_2$ value that delivers the highest classification accuracy indicated in Table 2.

Figure 2 shows that our approach can produce models with a low number of features just sacrificing a little bit the classification performance. This is what happens, for instance, for the breast data set, where just 4 features out of 30 are needed to attain a 97% of accuracy, and for the database diabetes, where
the use of the most relevant feature only entails a decrease of less than 2% in the prediction ability. The results for the databases colorectal and lymphoma, with a substantially larger number of features, are also remarkable. Indeed, the best accuracy result is attained in the colorectal database just considering the 10 most relevant features out of 2000, whereas only around a 1% of the total amount of features (40 out of 4026) are necessary to obtain a 96.87% of well-classified elements in the lymphoma data set.

5.3. Interpretability of the results

To evaluate the interpretability of $MM - FS$ we compare in Table 3 the five most important features that our approach identifies with respect to the relevant features pinpointed in the technical literature. In the case of our approach, the features are presented according to their relevance. For instance, for the breast data set, features radius_worst and texture_worst are the most and the second most important features. We have included a reference between parentheses to the benchmark approach used for all databases, except for lymphoma since no article reports the most relevant features for this database.

| MM-FS        | breast         | diabetes      | lymphoma      | colorectal   |
|--------------|----------------|---------------|---------------|--------------|
|              | radius_worst,  | glucose,      | 3783, Hsa.36689, |
|              | texture_worst, | body_mass_index, | 461, Hsa.1660, |
|              | smoothness_worst, | pregnancies, | 2267, Hsa.8147, |
|              | symmetry_worst, | diabetes_pedigree, | 2251, Hsa.6814, |
|              | concave_points_worst, | blood_pressure | 512, Hsa.41260 |

| Bench        | breast         | diabetes      | lymphoma      | colorectal   |
|--------------|----------------|---------------|---------------|--------------|
|              | radius_worst,  | glucose,      | 3783, Hsa.36689, |
|              | texture_worst, | body_mass_index, | 461, Hsa.1660, |
|              | smoothness_worst, | pregnancies, | 2267, Hsa.8147, |
|              | symmetry_worst, | diabetes_pedigree, | 2251, Hsa.6814, |
|              | concave_points_worst, | blood_pressure | 512, Hsa.41260 |
| (Ref. [15]) | (Ref. [34])   | (Ref. [23])   |               |              |

Table 3: Comparison of the selected features in the $MM$ approach and some benchmark approaches from the technical literature.

We can observe in Table 3 that most of the features that our methodology identifies as relevant are also deemed as significant in the technical literature. In the case of the breast data set, besides identifying already known important features, [15], our approach also considers as relevant features smoothness_worst...
and symmetry_worst. Something similar happens in the data set diabetes, where features glucose, body_mass_index and diabetes_pedigree among others are selected to be relevant for determining whether a new patient suffers from diabetes or not. This conclusion coincides with the one obtained in the literature, [34]. Finally, the model here proposed is able to found 2 of the genes which have been detected in the literature, [23], to be important in the diagnosis of colon cancer out of the 2000 features available in the data set colorectal. Apart from this information, the MM-FS methodology also selects three more relevant genes.

Hence, our proposal is competitive compared to benchmark methodologies, not only in terms of classification accuracy and feature ranking, as Sections 5.1 and 5.2 respectively show, but also in terms of interpretability.

6. Conclusions and Future Work

This paper deals with the problem of feature selection in nonlinear SVM classification. To this aim, a novel embedded feature selection approach is proposed, by means of a min-max optimization problem that seamlessly balances model complexity and classification accuracy. Unlike existing ad-hoc approaches, the proposed model can be efficiently solved with standard off-the-shelf optimization software, thanks to an equivalent reformulation that leverages duality optimization theory.

Numerical experience shows that our feature selection approach is able to select and rank the features in terms of their predictive power, preserving similar out-of-sample accuracy results than the classification performance obtained when all the features are considered. Besides, numerical tests with various databases show that the proposed approach significantly outperforms state-of-the-art embedded methods for feature selection when solved with off-the-shelf software and is comparable to them when these are solved using ad-hoc strategies. Finally, our approach produces interpretable classification models and correctly identify the relevant features reported in the literature.

In this paper, we have restricted ourselves to the Gaussian kernel. Nevertheless, the model here proposed can be extended to other families of kernels,
such as polynomial or sigmoid in a straightforward manner. In addition, the extension of our proposal to other Data Science problems, e.g., regression or clustering, or to other real-world applications, for instance, for power system operations, deserves further study.

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