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Support Vector Machines with Constraints for Sparsity in the Primal Parameters

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Abstract—This paper introduces a new support vector 1 machine (SVM) formulation to obtain sparse solutions in the 2 primal SVM parameters, providing a new method for feature 3 selection based on SVMs. This new approach includes additional 4 constraints to the classical ones that drop the weights associated 5 to those features that are likely to be irrelevant. A v-SVM 6 formulation has been used, where ν indicates the fraction of features to be considered. This paper presents two versions of 8 the proposed sparse classifier, a 2-norm SVM and a 1-norm SVM, 9 the latter having a reduced computational burden with respect to 10 the first one. Additionally, an explanation is provided about how 11 12 the presented approach can be readily extended to multiclass classification or to problems where groups of features, rather 13 than isolated features, need to be selected. The algorithms have 14 been tested in a variety of synthetic and real data sets and they 15 have been compared against other state of the art SVM-based 16 linear feature selection methods, such as 1-norm SVM and doubly 17 regularized SVM. The results show the good feature selection 18 ability of the approaches. 19

Index Terms—Feature group selection, feature selection,
 margin maximization, multiclass classification, support vector
 machines.

I. INTRODUCTION

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UPPORT vector machines (SVMs) [1], [2] are considered 24 the state-of-art in machine learning due to their well 25 known good performance in a wide range of applications 26 [3]-[5]. The SVM criterion minimizes a loss term, called hinge 27 loss, plus an additional quadratic penalization term which 28 regularizes the solution [6]. This hinge loss minimization 29 allows SVMs to approximate Bayes' rule without estimating 30 the conditional class probability [7] and makes it converge to 31 a maximum margin solution [8], thus endowing SVMs with 32 good generalization properties. 33

In spite of the generally good performance of SVMs, in many practical situations, useless, redundant, or noisy features can degrade the attained solution. The reason for this is that

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the SVM solution is based on a combination of all input features, including the irrelevant ones. As it is stated in the bet-on-sparsity principle [9], this situation is undesired and it would be preferable to obtain a solution consisting only of the relevant features. That way, more accurate and interpretable solutions can be achieved.

To achieve this goal, a feature selection process [10], [11] is 43 usually applied. Classical feature selection techniques, such as 44 filtering [12] or wrapping [13], [14] approaches, are used as an 45 independent preprocessing step before the training of the final 46 classification (or regression) machine. More recent feature 47 selection methods combine the feature selection process with 48 the final predictor training. For instance, in [15]-[17] an 49 objective function that combines an accuracy prediction term 50 with a term associated to the sparsity in the number of selected 51 variables is employed. In [18]–[20] the SVM prediction output 52 is considered as a linear combination of kernel functions and 53 then, the prediction accuracy is evaluated as a function of the 54 used and discarded features. This method, known as recursive 55 feature elimination (RFE), has been widely employed for SVM 56 classification, however, recent works [21] have shown that 57 RFE is not consistent with maximum margin solutions. 58

In contrast to the approaches that include an explicit fea-59 ture selection strategy (either independent or combined with 60 the classification step), classifiers directly providing sparse 61 solutions are usually preferred. Following this point of view, 62 the LASSO method was proposed in [15]. LASSO includes a 63 1-norm regularization term in the optimization problem. Since 64 this norm has a singularity at the origin, some coefficients of 65 the solution vector are shrunk to zero, what provides sparse 66 solutions. Since then, many researchers have focused their 67 work on minimizing 1-norm penalized functions [22]-[24]. 68 In fact [25] points out the need and usefulness of linear sparse 69 solutions in problems like functional magnetic resonance 70 imaging. 71

In [26], the classical SVM formulation is modified by replacing the quadratic penalization term with a 1-norm penalty, what leads to solutions with sparse coefficients. Although this SVM formulation can only be used for feature selection in linear classification problems, this approach has nevertheless been successfully used in a large number of applications, such as computational biology [27], [28], drug-design [17] or gene microarrays classification [29], among others.

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Although 1-norm SVMs retain most of the desired properties of classical SVMs, such as margin maximization, they may fail to provide good solutions in certain situations. As it is

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usually outperform their 1-norm counterparts. Furthermore, as 85 it is pointed out in [30] and [31], the 1-norm SVM presents two 86 additional limitations: first, when there are highly correlated 87 variables, it usually removes some of them, and, second, the 88 maximum number of selected features is limited by the number 89 of available training data. Trying to overcome these draw-90 backs, elastic nets [32] and their particularization to SVMs 91 by means of the doubly regularized support vector machine 92 (Dr-SVM) [30], [31] are proposed, this new approach gener-93 alizes the LASSO and 1-norm SVM methods by keeping the 94 2-norm regularization term and including an additional 1-norm 95 penalty term to force sparsity. Despite common improved 96 performance of Dr-SVM, both 1-norm and Dr-SVMs are not 97 suitable methods when the underlying model is truly sparse, 98 since they are not able to remove all unnecessary variables 99 from the final classifier, this problem was already remarked 100 for 1-norm SVMs in [33] and, in the experimental section of 101 this paper, we will illustrate it for Dr-SVM. 102

An additional limitation of 1-norm SVM and Dr-SVM, is 103 that they are not well suited to multiclass classification or 104 to problems where features have to be selected or removed 105 using predefined groups. One possible solution could consist 106 in adding a group LASSO [34] or an ∞ -norm [35] penaliza-107 tion term into the SVM formulation. However, both options 108 result in a more complex SVM formulation, which cannot be 109 solved with standard linear programming (LP) or quadratic 110 programming (QP) solvers. 111

In this paper, a new SVM formulation for the linear case 112 is presented that directly forces sparse solutions. Rather than 113 modifying the objective function, additional constraints are 114 included in the minimization task in order to identify irrelevant 115 features and to drop their associated weights to values lower 116 than a small parameter ε . This constant can be adjusted during 117 the optimization problem resolution by predefining the number 118 of relevant features to be kept in the final solution using a 119 ν -SVM formulation [36]. We will show that these additional 120 constraints can be incorporated to force sparsity in both 121 2-norm and 1-norm SVM formulations. Our approach allows 122 to overcome the limitations of 1-norm SVMs and Dr-SVMs 123 in different ways. First, by properly adjusting parameter ν , 124 the algorithm is able to remove all irrelevant features from 125 the final model. Second, the proposed formulation can be 126 applied to the selection of isolated features or predefined 127 feature groups where needed. Finally, as it will be shown in 128 the experiments section, more accurate solutions are usually 129 achieved, particularly, when using the new constraints together 130 with the 2-norm SVM. 131

The rest of this paper is organized as follows. In the next 132 section, we introduce our approach to force feature selection 133 in SVM classifiers, explaining how it can be applied both to 134 2-norm and 1-norm formulations. Section III presents some 135 extensions of the method to address the selection of features 136 in predefined groups of variables, as well as for multiclass 137 classification problems. Section IV presents extensive simu-138 lation work to illustrate the performance of our approach, 139 and its advantages with respect to previous proposals for 140

feature selection in SVMs. Finally, Section V presents the 141 main conclusion of our work, and identifies some lines for 142

II. SVM WITH EXPLICIT CONSTRAINTS FOR 144 FEATURE SELECTION

A. Problem Overview

In this paper, we consider classification problems where 147 the representation of the input data contains some features, 148 which are irrelevant for the task at hand. This may happen 149 as a consequence of redundancy between the input variables 150 or, simply, because some of the input features do not carry 151 any valuable information for the classification. In a standard 152 machine learning setup, we are given a set of N training 153 labeled data, $S = {\mathbf{x}^{(l)}, y^{(l)}}, l = 1, \dots, N$, where $\mathbf{x}^{(l)} \in$ 154 \Re^d are the input vectors and $y^{(l)}$ are used to encode class 155 membership, from which we have to learn both the subset of 156 relevant input variables and the classification function itself. 157

Linear classifiers obtain their outputs according to a thresh-158 olded version of the estimator 159

$$\hat{\mathbf{y}} = \mathbf{w}^T \mathbf{x} + b \tag{1}$$
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where \hat{y} is the output of the classifier for input vector **x**, 161 \mathbf{w} is the vector that defines the classifier, and b is a bias 162 term. For the SVM case, the Representer's Theorem [1], [2] 163 states that the solution vector will lie in the subspace spanned 164 by all training vectors $\{\mathbf{x}^{(l)}\}$. When irrelevant features are 165 present in the data we can carry out a pre-processing stage to 166 select the most informative variables or, alternatively, discard 167 the variables x_i whose associated weight w_i is exactly zero 168 after the optimization of the classifier. However, since noise is 169 normally present in the data, none of the components of w will 170 be exactly zero unless sparsity is included as an optimization 171 criterion during the training of the classifier. 172

A standard way to impose sparsity in w is to include 173 a regularization term in the cost function, based on the 174 1-norm of **w**, i.e., $\|\mathbf{w}\|_1 = \sum_i |w_i|$. This regularizer presents 175 singularity points whenever any of the components of w is 176 zero, what tends to nullify some of the solution weights, thus 177 favoring sparse solutions. However, this mechanism does not 178 necessarily imply that all weight components associated to 179 irrelevant variables will become zero [33]. 180

Rather than modifying the structural risk term in the SVM 181 functional, in this paper, we propose a new approach to impose 182 sparsity in the solution by introducing a set of additional 183 constraints for the optimization problem. We will see that 184 our method is able to automatically identify all irrelevant 185 features, thus constituting an effective mechanism for imple-186 menting SVMs that incorporate a feature selection approach. 187 Furthermore, since the 2-norm regularization term can still be 188 used, this usually results in a better performance when the true 189 underlying solution is non sparse. 190

B. 2-Norm SVMs with Sparsity Constraints

Classical SVMs are based on the minimization of a func-192 tional that includes two terms. The first term is the squared 193 norm of the weight vector \mathbf{w} , which is inversely proportional 194

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to the margin of classification [1], thus, this term is related
to the structural risk of the classifier and to its generalization
capabilities. The second term in the objective functional, which
is known as the empirical risk term, is a sum of errors over
the training data. In other words, the linear SVM problem can
be stated as

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min
$$\|\mathbf{w}\|^{2} + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)}$$

s.t. $y^{(l)} (\mathbf{w}^{T} \mathbf{x}^{(l)} + b) \ge 1 - \xi^{(l)}; \quad \forall l$
 $\xi^{(l)} \ge 0; \quad \forall l$ (2)

where slack variables $\xi^{(l)}$ are introduced to allow some of the training patterns to be misclassified or to lie inside the classifier margin, and where *C* is a constant that controls the trade-off between the structural and empirical risk terms.

As it is well known, this optimization method provides a sparse solution in the sense that **w** is a linear combination of only a subset of the training data [the so-called support vectors (SVs)]. However, if feature selection is pursued during the optimization, a solution sparse in the parameters **w** is needed. In order to obtain such a solution, we will introduce some additional constraints in the optimization problem.

We start by rewriting each of the weight components, 213 $w_i, i = 1, \dots, d$, as $w_i = u_i - v_i$, with $u_i, v_i \ge 0$. As 214 we will explain later, our optimization problem will implicitly 215 enforce that at least one of the two terms in the subtraction, 216 u_i or v_i , is zero, depending on whether the optimal weight is 217 positive $(u_i > 0 \text{ and } v_i = 0)$, negative $(u_i = 0 \text{ and } v_i > 0)$ or 218 zero $(u_i = v_i = 0)$. Therefore, the square norm of the weight 219 vector is given, in terms of these new variables, by 220

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$$\|\mathbf{w}\|_{2}^{2} = \sum_{i=1}^{d} u_{i}^{2} + v_{i}^{2}.$$
 (3)

Furthermore, in order to obtain a sparse solution in w, we introduce some additional constraints to upper bound the absolute value of weight components by a small constant ε , i.e., $|w_i| = u_i + v_i < \varepsilon$. Introducing (3) and the new constraints into (2), we get the following modified SVM formulation:

$$\min \sum_{i=1}^{d} (u_i^2 + v_i^2) + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)} + \frac{C'}{d} \sum_{i=1}^{d} \gamma_i$$
s.t. $y^{(l)} \left[\sum_{i=1}^{d} (u_i - v_i) x_i^{(l)} + b \right] \ge 1 - \xi^{(l)}; \quad \forall l$
 $\xi^{(l)} \ge 0; \quad \forall l$
 $u_i + v_i \le \varepsilon + \gamma_i; \quad \forall i$
 $u_i, v_i \ge 0; \quad \forall i$
 $\gamma_i \ge 0; \quad \forall i.$

$$(4)$$

Although the above optimization problem has not explicitly included, the constraint $u_i v_i = 0$, (4) is indirectly forcing that either u_i or v_i is equal to 0. Note that among all possible pairs of values (u_i, v_i) that are able to provide a certain value w_i , the pair which minimizes $\sum_{i=1}^{d} (u_i^2 + v_i^2)$ has to fix either u_i or v_i to 0, for instance, for positive w_i and according to its definition in terms of u_i and v_i , minimization of the functional in (4) will lead to $v_i = 0$ and $u_i = w_i$. The opposite situation will occur for $w_i < 0$.

Note that in our redefinition of the problem we have 237 introduced new slack variables γ_i and those slack variables 238 associated with relevant features will be greater than zero after 239 the functional optimization. Thus, these constants need to be 240 introduced in the objective functional weighted with a trade-241 off parameter C'. The above minimization problem can be 242 directly solved in the primal over the variables u_i , v_i , b, γ_i , 243 and $\xi^{(l)}$, using standard QP algorithm. 244

We can now get some insight into the sparsity mechanism 245 that has been adopted. If irrelevant features are present in the 246 input representation space, most classification schemes would 247 still assign them a non zero weight w_i due to the noise present 248 in the data. However, if a w_i value greater than ε were assigned 249 in our scheme, γ_i would be strictly positive, increasing the 250 value of the functional. Thus, on the one hand irrelevant 251 features that do not significantly decrease the empirical error 252 term will simply be assigned weights smaller, in absolute 253 terms, than ε . On the other hand, components w_i which are 254 necessary to define the SVM solution will have values larger 255 than ε . It is straightforward to use the values of slacks γ_i after 256 the optimization to check whether a variable has been removed 257 or incorporated into the classification model. 258

This new SVM with sparsity constraints performs feature 259 selection on the input variables, so we will hereafter refer to 260 it as sparse primal support vector machine (SP-SVM). 261

At first sight, one could think that the sparsity constraints in 262 (4) are equivalent to a 1-norm penalty term and thus algorithm 263 (4) is equivalent to Dr-SVM. Nevertheless, these constraints 264 have been introduced here through an ε -insensitive cost func-265 tion. As we will analyze along this paper, this new formulation 266 provides two advantages: 1) the sparsity of the model can be 267 easily adjusted by the user through a v SVM formulation, 268 and 2) extensions of this model to group feature selection and 269 multiclass problems are straightforwardly derived. 270

The computational cost of (4) is larger than that of 271 1-norm or Dr-SVMs due to the new constrains. However, an 272 efficient implementation of the problem, which exploits the 273 sparse formulation of these constrains, it results in a very 274 moderate computational increase. 275

Finally, it is important to point out that a major limitation of problem (4), as well as 1-norm and Dr-SVM algorithms, is their linear formulation. Note that their non linear extension would provide a non linear boundary with a kernel selection mechanism, instead of an automatic feature selection criterion.

C. 2-Norm v-SP-SVM

In this section, we introduce a modification of the SP-SVM formulation in (4) to automatically adjust the value of ε , following the ν -SVM that was introduced in [36]. In this formulation of the SVM, ε is traded off against model complexity and slack variables through a constant $\nu \in (0, 1]$. Then, the optimization problem to solve is given by 287

$$\min \quad \sum_{i=1}^{d} (u_i^2 + v_i^2) + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)} + C' \left[v\varepsilon + \frac{1}{d} \sum_{i=1}^{d} \gamma_i \right] \qquad _{288}$$

s.t.
$$y^{(l)} \left[\sum_{i=1}^{d} (u_i - v_i) x_i^{(l)} + b \right] \ge 1 - \xi^{(l)}; \quad \forall l$$

$$\xi^{(l)} \ge 0; \quad \forall l$$

$$u_i + v_i \le \varepsilon + \gamma_i; \quad \forall i$$

$$u_i, v_i \ge 0; \quad \forall i$$

$$\gamma_i \ge 0; \quad \forall i$$

$$\varepsilon \ge 0.$$

(5)

As above, this optimization problem can be directly solved in 290 the primal, with respect to variables u_i , v_i , b, γ_i , $\xi^{(l)}$, and ε . 291 It is well known [36] that, when the standard ν support 292 vector regression is applied resulting a non zero ε , ν is an 293 upper bound on the fraction of errors and a lower bound on 294 the fraction of SVs. Note that in (5), if the dual formulation of 295 the problem was used and we let $\{\beta_i\}_{i=1}^d$ be the dual variables 296 associated to the sparsity constraints, the following equalities 297 had to be verified: 298

 $\sum_{i=1}^{d} \beta_i \le \frac{C'}{d} \nu$

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$$0 \le \beta_i \le \frac{C'}{d}$$

what forces v to be an upper bound of the number of dual 301 variables β_i taking a value of C'/d, that is, ν is an upper 302 bound over the number of slack variables γ_i different from 0. 303 This leads to a useful result for the proposed ν -SP-SVM: ν 304 is an upper bound on the fraction of components of \mathbf{w} whose 305 absolute value is less than ε . In other words, parameter ν can 306 be used to control the sparsity of the solution, setting a priori 307 the maximum number of features that can be selected by the 308 2-norm v-SP-SVM. 309

310 D. 1-Norm v-SP-SVM

Using the 1-norm of w in the structural risk term of 311 classical SVMs leads to LP problems, which have a reduced 312 computational burden when compared to the QP formulation 313 required for 2-norm SVMs. Similar benefits can be obtained 314 for the SP-SVM proposed in the previous sections. Note that 315 the constraints that were imposed in order to force sparsity 316 do not affect the regularizer for w in any way, thus, in order 317 to extend either (4) or (5) to the 1-norm case, it is sufficient 318 to replace the structural risk term accordingly. For instance, 319 for the ν -SP-SVM in its 1-norm version this leads to 320

$$\min \sum_{i=1}^{d} (u_i + v_i) + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)} + C' \left[v\varepsilon + \frac{1}{d} \sum_{i=1}^{d} \gamma_i \right]$$

s.t.
$$y^{(l)} \left[\sum_{i=1}^{d} (u_i - v_i) x_i^{(l)} + b \right] \ge 1 - \xi^{(l)}; \quad \forall l$$
$$\xi^{(l)} \ge 0; \quad \forall l$$
$$u_i + v_i \le \varepsilon + \gamma_i; \quad \forall i$$
$$u_i, v_i \ge 0; \quad \forall i$$
$$\gamma_i \ge 0; \quad \forall i$$
$$\varepsilon > 0.$$
 (6)

Using LP optimization tools, this problem can be solved in a more efficient way than with QP optimizers, obtaining the values of u_i , v_i , and b that define the solution. As with the 2-norm formulation, the selected features will be those whose corresponding slacks γ_i are greater than zero.

III. SP-SVM EXTENSIONS

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In this section, we consider two different extensions of 328 our SVM with feature selection. First, we will consider the 329 joint selection (or removal) of features that are assigned to 330 predefined groups, second, we will study how the SP-SVM can 331 be extended to multi-class problems. During our derivations in 332 this section, we will only consider the ν -SP-SVM formulation 333 with 2-norm for the regularization term, although it would 334 be straightforward to apply similar extensions to the standard 335 SP-SVM or 1-norm v-SP-SVM. 336

A. v-SP-SVM with Feature Selection Over Predefined Groups 337

In some practical situations, variables can appear grouped 338 together in predefined sets that can be jointly relevant or 339 irrelevant. Then, the feature selection process must be applied 340 over these sets rather than over the isolated features. This 341 is for instance the case when encoding categorical variables 342 with binary words. Either all binary variables corresponding 343 to the same categorical feature should be selected or removed 344 together. 345

Let us assume that the input features are structured in G < d346 disjoint groups, i.e., each input feature belongs to exactly 347 one group. Let us also denote by S_g the indexes of the g-th 348 group of variables, with $g = 1, \ldots, G$. Then, we can modify 349 (5) by replacing the constraints over the absolute values of 350 each individual weight (i.e., $u_i + v_i \le \varepsilon + \gamma_i$) by alternative 351 constraints each one consisting of the sum of absolute values 352 of all weights corresponding to the variables belonging to the 353 same group 354

$$\min \sum_{i=1}^{d} (u_i^2 + v_i^2) + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)} + C' \left[v\varepsilon + \frac{1}{G} \sum_{g=1}^{G} \gamma_g \right]$$
s.t.
$$y^{(l)} \left[\sum_{i=1}^{d} (u_i - v_i) x_i^{(l)} + b \right] \ge 1 - \xi^{(l)}; \quad \forall l$$

$$\xi^{(l)} \ge 0; \quad \forall l \qquad (7) \quad {}_{355}$$

$$\sum_{i \in S_g} u_i + v_i \le \varepsilon + \gamma_g; \quad \forall g$$

$$u_i, v_i \ge 0; \quad \forall i$$

$$\gamma_g \ge 0; \quad \forall g$$

$$\varepsilon > 0$$

where γ_g are slacks associated to each group and γ_g values greater than 0 after optimization indicate, which groups have been selected and included in the classification model. Now, parameter ν can be used to *a priori* establish the maximum number of groups that should be selected by the algorithm, thus providing a control mechanism for adjusting the degree of sparsity desired for the solution.

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Finally, it is important to point out some advantages of this formulation with regard to other reference methods.

- 1) The standard formulation of 1-norm SVMs [26] cannot be used for feature selection in the setup that we have studied here. This is due to the fact that standard 1-norm SVM directly introduces term $||\mathbf{w}||_1$ in the objective function to force sparsity, making it impossible to force all coefficients of the same group to shrink to zero at the same time.
- 2) Forcing sparsity over groups with a group LASSO 372 penalty term [34] precludes the standard SVM formu-373 lation, since it turns it out into a non linear convex 374 optimization problem. Feature selection over groups 375 only implies a modification of the introduced con-376 straints due to the fact that our approach forces spar-377 sity by means of additional constraints; therefore, stan-378 dard LP or QP optimizers can be used to solve the 379 problem. 380
- 3) Furthermore, if 1-norm were used to penalize weights
 coefficients in the functional of (7), not only groups
 selection would be implemented, but also sparsity within
 the groups would be favored.

385 B. Multiclass v-SP-SVM

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Here, we present the extension to multiclass classification problems by following the SVM multiclass approach from [37]. Let us consider a classification problem with *K* classes. Then, in this case we have $y^{(l)} \in \{1, ..., K\}$. Accordingly, the classification function for a linear classifier is given by

$$\hat{y} = \arg \max_{k=1,\dots,K} \mathbf{w}_k^T \mathbf{x} + b_k \tag{8}$$

i.e., *K* different outputs associated to each class are computed, and then the pattern is classified according to the largest output. The set of vectors and bias terms $\{\mathbf{w}_k, b_k\}, k =$ $1, \ldots, K$, which define the classifier can be obtained as the solution to the following optimization problem:

$$\min \sum_{k=1}^{K} \|\mathbf{w}_{k}\|^{2} + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)}$$

s.t. $\left[\mathbf{w}_{y^{(l)}}^{T} \mathbf{x}^{(l)} + b_{y^{(l)}}\right] - \left[\mathbf{w}_{m}^{T} \mathbf{x}^{(l)} + b_{m}\right] \ge 2 - \xi^{(l)};$ (9)
 $\forall l; \ m \neq y^{(l)}$
 $\xi^{(l)} > 0 \quad \forall l.$

As with the binary SVM, the objective function consists of the 399 sum of two terms that are related to the structural and empirical 400 risks. The constraints for the minimization try to force that, 401 for each training sample, the largest output of the system is 402 obtained for the correct class. Otherwise, slack variable $\xi^{(l)}$ 403 will take a value equal to the distance between the largest 404 output and the output associated to the actual class of the 405 pattern [37]. 406

We can now introduce sparsity constraints to allow feature selection during the training of the multiclass SVM. A straightforward extension of our strategy for the binary case would lead to

$$\min \sum_{k=1}^{K} \sum_{i=1}^{d} (u_{k,i}^{2} + v_{k,i}^{2}) + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)} + C' \left[v\varepsilon + \frac{1}{Kd} \sum_{k=1}^{K} \sum_{i=1}^{d} \gamma_{k,i} \right] \text{s.t.} \left[\sum_{i=1}^{d} (u_{y^{(l)},i} - v_{y^{(l)},i}) x_{i}^{(l)} + b_{y^{(l)}} \right] - \left[\sum_{i=1}^{d} (u_{m,i} - v_{m,i}) x_{i}^{(l)} + b_{m} \right] \ge 2 - \xi^{(l)}; \forall l; \ m \neq y^{(l)} \xi^{(l)} \ge 0; \quad \forall l u_{k,i} + v_{k,i} \le \varepsilon + \gamma_{k,i}; \quad \forall i; \ \forall k u_{k,i}, v_{k,i} \ge 0; \quad \forall i; \ \forall k \gamma_{k,i} \ge 0; \quad \forall i; \ \forall k \varepsilon \ge 0$$
 (10)

where we have defined $\mathbf{w}_k = \mathbf{u}_k - \mathbf{v}_k$, and $u_{k,i}$ and $v_{k,i}$ are the *i*-th components of \mathbf{u}_k and \mathbf{v}_k , respectively.

The above formulation would result in vectors \mathbf{w}_k with 414 different sparsity distributions. It should be noted, however, 415 that in order to perform a true feature selection, it would be 416 necessary that the irrelevant features are removed from all 417 \mathbf{w}_k at the same time. In other words, to discard a feature 418 x_i from the final classification model, it is necessary that 419 such a feature is simultaneously ignored for the computation 420 of all K system outputs. In order to do so, we can use an 421 approach similar to that in Section III-A, including in a single 422 constraint all weights $u_{k,i}$ and $v_{k,i}$ associated to the same 423 feature. Proceeding in this way, (10) is changed into 424

$$\min \sum_{k=1}^{K} \sum_{i=1}^{d} (u_{k,i}^{2} + v_{k,i}^{2}) + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)}$$

$$+ C' \left[v\varepsilon + \frac{1}{d} \sum_{i=1}^{d} \gamma_{i} \right]$$
s.t.
$$\left[\sum_{i=1}^{d} (u_{y^{(l)},i} - v_{y^{(l)},i}) x_{i}^{(l)} + b_{y^{(l)}} \right]$$

$$- \left[\sum_{i=1}^{d} (u_{m,i} - v_{m,i}) x_{i}^{(l)} + b_{m} \right] \ge 2 - \xi^{(l)}; \quad \forall l; \ m \neq y^{(l)}$$

$$\xi^{(l)} \ge 0; \quad \forall l$$

$$\sum_{k=1}^{K} u_{k,i} + v_{k,i} \le \varepsilon + \gamma_{i}; \quad \forall i$$

$$u_{k,i}, v_{k,i} \ge 0; \quad \forall i; \forall k$$

$$\gamma_{i} \ge 0; \quad \forall i$$

$$\varepsilon \ge 0.$$

$$(11)$$

The above problem can be solved using QP optimizers. At the solution, those features with an associated $\gamma_i > 0$ will be selected, while all the rest are excluded from the classifier.

TABLE I

CE RATES AND NUMBER OF FEATURES PROVIDED IN THE ORANGE DATA PROBLEM BY THE DIFFERENT METHODS UNDER STUDY: STANDARD 2 AND 1-NORM SVMS, Dr-SVM and 2 and 1-NORM *v*-SP-SVMS. PARAMETERS *q* and *p* INDICATE THE NUMBER OF RANDOM FEATURES INCLUDED IN THE DATA SET AND THE TOTAL NUMBER OF FEATURES IN THE EXPANDED INPUT SPACE, RESPECTIVELY

a n		Standar	d SVM	Dr-SVM	v-SP-	SVM
<i>q</i> , <i>p</i>		2-norm	1-norm	DI-5 V WI	2-norm	1-norm
0, 5	CE	7.87(±2.15)	7.30(±1.18)	7.30(±1.08)	6.89(±1.08)	6.89(±1.07)
0, 5	# feat.	-	4.46(±0.93)	4.75(±0.63)	2.66(±0.94)	2.67(±0.91)
2, 14	CE	10.56(±2.50)	8.16(±1.18)	8.42(±1.39)	6.78(±1.16)	6.81(±1.15)
2, 14	# feat.	-	6.34(±3.40)	7.46(±3.30)	2.45(±1.28)	2.27(±0.88)
4, 27	CE	13.83(±2.88)	8.71(±1.39)	8.84(±1.60)	6.88(±1.28)	6.91(±1.36)
4, 27	# feat.	-	6.49(±4.65)	9.79(±3.26)	2.48(±1.35)	2.27(±0.87)
6, 44	CE	15.89(±3.01)	8.75(±1.34)	9.19(±1.61)	6.64(±1.23)	6.74(±1.34)
0, 44	# feat.	-	6.41(±4.93)	13.56(±3.79)	2.36(±1.65)	2.44(±1.47)
8, 65	CE	18.81(±2.92)	8.93(±1.49)	10.05(±2.07)	6.76(±1.37)	6.85(±1.47)
0, 05	# feat.	-	6.22(±4.21)	18.63(±5.02)	2.27(±1.21)	2.38(±1.42)
12, 119	CE	23.59(±2.83)	8.80(±1.16)	11.11(±2.94)	6.64(±1.24)	6.70(±1.22)
12, 119	# feat.	-	7.60(±3.04)	25.44(±8.41)	2.15(±1.27)	2.21(±1.32)
16, 189	CE	27.18(±2.65)	8.98(±1.40)	12.86(±3.54)	6.84(±1.30)	6.97(±1.34)
10, 109	# feat.	-	10.00(±4.65)	34.81(±8.49)	2.53(±2.10)	2.56(±1.80)

As before, parameter ν can be used to control the maximum 429 number of features to be selected by the multiclass ν -SP-SVM. 430 Similarly to what we explained for the group selection case, 431 imposing sparsity through additional constraints is key in order 432 to perform a common feature selection for all classification 433 problems, and approaches relying on the introduction of 434 1-norm penalties in the objective function would either fail to 435 select the same features for all classification tasks, or preclude 436 the use of standard LP or QP optimizers. 437

IV. EXPERIMENTS

In this section, we will test the performance of the proposed 2 and 1-norm ν -SP-SVM algorithms. For this purpose, we will analyze both the provided classification error (CE) rate and the number of selected features compared to those of standard 2 and 1-norm SVMs, as well as the Dr-SVM from [30].

In all experiments, free SVM parameters have been opti-444 mized through a cross validation (CV) process. Parameter C445 of standard SVMs has been logarithmically swept with 10 446 values from 10⁻²N to 10⁶N, N being the number of training 447 data. Parameter C of ν -SP-SVMs has been explored with 5 448 values in the same range. For each value of C, C' has been 449 swept in the set of values: $\{0.01C, 0.1C, C, 10C, 100C\}$. In 450 order to evaluate the influence of v in the number of selected 451 features, we have considered the overall set of values v = i/d, 452 1 < i < d, where d is the data dimension, when v-SP-453 SVM is applied over a predefined feature group, parameter 454 d is replaced by the number of groups G. As for Dr-SVM 455 parameters, λ_1 and λ_2 , they have been selected among the set 456 of values {0.01, 0.1, 1, 10, 100}. 457

In the following discussions, both results evaluating the evolution of the CE and the number of features when ν value is explored, and results achieved when ν value is cross validated, will be analyzed. Additionally, we will include the CE achieved by a new SVM retrained with only the subset of features selected by the ν -SP-SVM methods, in this way, we will check whether the fact of pruning the weights associated to irrelevant features degrades the final model performance. 463

The MOSEK library¹ has been used as optimizer for all 466 algorithms under study.

A. Orange Data Model

As a first simulation problem, we have considered the 469 "orange data" model, which has been previously employed 470 in [29] to test the standard 1-norm SVM performance. In this 471 problem, two standard normal independent random variables 472 x_1, x_2 are generated. Negative class elements of data $[x_1, x_2]^T$ 473 satisfy inequality 4.5 $\leq x_1^2 + x_2^2 \leq 8$, whereas positive 474 elements are distributed along all space \mathbb{R}^2 . Thus, negative 475 class surrounds almost all positive class patterns, like the 476 skin of an orange. Additionally, to check the feature selection 477 ability of the different algorithms, q random independent 478 standard Gaussian inputs have been included in the model. 479 Finally, this input space has been expanded with a second 480 degree polynomial function, i.e., $\{\sqrt{2}x_j, \sqrt{2}x_jx_k, x_j^2, j, k =$ 481 $1, 2, \ldots, 2 + q$ to create a new data set with p new input 482 features. 483

In the experiments, the number of added random features, *q*, has been fixed to 0, 2, 4, 6, 8, 12, and 16 generating an expanded input space of 5, 14, 27, 44, 65, 119, and 189 features. To design the different SVM classifiers, independent and balanced training, validation and test data sets have been generated with 100, 500, and 1000 data, respectively, and each simulation has been repeated 200 times. In this experiment,

²Note that the Bayes boundary is given by $x_1^2 + x_2^2 = 4.5$, therefore, from the overall set of *p* new features, only terms x_1^2 and x_2^2 are useful.

¹MOSEK ApS, Denmark. Available at http://www.mosek.com. The MOSEK Optimization Tools version 6.0 (Revision 61). User's manual and reference, 2010.

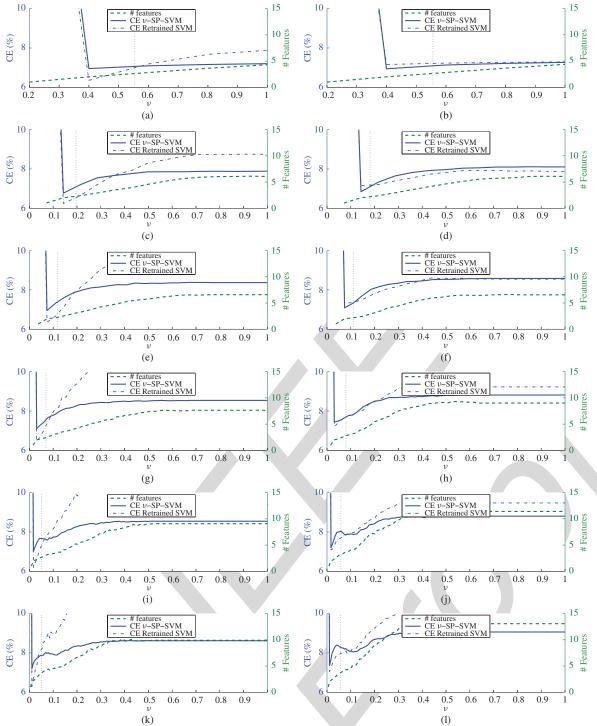


Fig. 1. Evolution of the averaged CE and the averaged number of selected features in ν -SP-SVM methods as a function of ν for orange data set. Dash-dotted line shows the averaged CE of an SVM retrained with the features selected by v-SP-SVM. Dotted vertical line marks the averaged cross-validated v value. (a) 2 norm v-SP-SVM (q = 0). (b) 1 norm v-SP-SVM (q = 0). (c) 2 norm μ -SP-SVM (q = 2). (d) 1 norm v-SP-SVM (q = 2). (e) 2 norm v-SP-SVM (q = 4). (f) 1 norm v-SP-SVM (q = 4). (g) 2 norm v-SP-SVM (q = 8). (h) 1 norm v-SP-SVM (q = 8). (i) 2 norm v-SP-SVM (q = 12). (j) 1 norm ν -SP-SVM (q = 12). (k) 2 norm ν -SP-SVM (q = 16). (l) 1 norm ν -SP-SVM (q = 16).

different SVM free parameters (C, C', and ν) have been 491 optimized using the validation set. 492

The MATLAB code that implements the proposed ν -SP-493 SVM algorithms and a demo, which allows us to replicate 494 the results shown in this section can be downloaded from 495 http://www.tsc.uc3m.es/ hmolina/paper_nu-SP-SVM/. 496

Table I presents the averaged CE rates achieved by the dif-497 ferent SVM methods under study and the number of features in their models. These results show the following.

1) Classical SVM methods rise the CE rate and the number 500 of features in the model when q is increased, as it is 501 expected, standard 1-norm SVM and Dr-SVM provide 502

sparser solutions than standard 2-norm SVM, even if 503 some noisy features are included in the final model. 504 Note that Dr-SVM, which penalizes with L1 and L2 505 norms, retains more useless features than 1-norm SVM 506 and, although its performance improves 2-norm SVM, 507 it is not as accurate as 1-norm SVM. 508

The proposed ν -SP-SVM approaches keep the classifi-509 cation error rates around 7%, independently of q and, 510 in most cases, they only employ the useful features: 511 note that the average number of selected features is 512 always very close to 2. However, standard 2-norm SVM 513 uses all original features and standard 1-norm SVM and 514 Dr-SVM tend to include some useless features. 515

3) When 2-norm and 1-norm v-SP-SVM results are com-516 pared to each other, we do not observe relevant differ-517 ences, since they present similar CEs and similar number 518 of features. 519

Fig. 1 depicts the evolution of the averaged classification 520 error and the averaged number of selected features as a 521 function of parameter ν in the orange problem, for each value 522 of ν , parameters C and C' have been adjusted by the validation 523 process. A dotted vertical line indicates the working point 524 of the results from Table I, when ν was also selected in 525 the validation process. Additionally, this figure includes the 526 averaged CE rate, which could be achieved by retraining a 527 new standard SVM with the set of features selected by ν -528 SP-SVMs. This figure shows the following behaviors of the 529 proposed methods. 530

1) As it was expected, ν plays a crucial role to obtain a 531 reduced number of features and an accurate solution. 532 Fixing $\nu = 1$, the provided results would be similar 533 to the standard 1-norm SVM, however, reducing v534 both performance improvements and reductions in the 535 number of model parameters could be achieved, mainly 536 if v was close to 2/d. 537

2) The role of ν as upper bound on the number of selected 538 features is clearly seen. When ν is close to 1, the 539 proposed v-SP-SVM methods do not include all original 540 features in their models, since most noisy features are 541 removed. For instance, when q = 8, 12, or 16, there 542 are 65, 119, and 189 original features, but v-SP-SVMs 543 employ less than 10, 12, or 14 features. 544

Finally, it is important to point out that the model 545 performance is not degraded by pruning the coefficients 546 associated to irrelevant features (those whose slack vari-547 ables γ_i are zero). If we compare the solutions provided 548 by ν -SP-SVM models with a new standard SVM trained 549 with the selected set of features, slight performance 550 improvements could be achieved; but, when any noisy 551 feature is included in the model, the retrained SVM tends 552 to overfit, whereas proposed v-SP-SVM models provide 553 accurate solutions. 554

B. Benchmark Data Sets 555

To test the performance of the proposed ν -SP-SVM clas-556 sifiers over real data sets, 8 benchmark binary classification 557 problems have been selected from the universal communica-558 tions identifier (UCI) repository [38]: Abalone, Credit, Hand, 559

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TABLE II

CHARACTERISTICS OF THE BINARY DATA SETS: NUMBER OF FEATURES AND NUMBER OF DATA BELONGING TO EACH CLASS IN TRAINING AND TEST SETS

Problem	# Features (<i>d</i>)	# Train samples (n_1/n_{-1})	# Test samples (n_1/n_{-1})
Abalone	8	1238/1269	843/827
Credit	15	215/268	92/115
Hand	62	1923/1900	906/891
Image	18	821/1027	169/293
Ionosphere	34	150/84	75/42
Pima	8	188/350	80/150
Spam	57	1218/1847	595/941
Wdbc	30	238/141	119/71

Image, Ionosphere, Pima, Spam, and Wisconsin Diagnostic 560 Breast Cancer (Wdbc). These problems have been chosen 561 because of their diversity in the number of data and dimen-562 sions. The main characteristics of these problems are summa-563 rized in Table II. To adjust the free parameters of the different 564 models, the parameter ranges described in the introduction of the experimental section have been swept by applying a fivefold CV process. 567

For this benchmark analysis we have also included, as 568 an additional reference method, the RFE method from [39]. 569 This algorithm carries out a feature selection process by 570 iteratively removing the feature with less weight in the SVM 571 solution. To fairly compare this method with proposed ν -SP-572 SVM methods, we have implemented the linear version of 573 the RFE algorithm, additionally, the final feature subset of the 574 RFE method is selected with a CV process (note that the RFE 575 method obtains a different feature subset in each iteration) and 576 a new SVM has been trained using only the selected features. 577

Table III shows the results achieved by the different SVM 578 algorithms under study averaged over 50 runs with randomly 579 selected training/validation sets. As it can be observed, stan-580 dard 1-norm SVM fails to remove irrelevant features in some 581 problems. For instance, in Abalone, Pima, and Spam almost 582 all original features are retained. Dr-SVM is worse than the 583 standard 1-norm SVM in this regard, and hardly removes 584 any feature in the considered problems (with the exception 585 of Credit). 586

In contrast, it is possible to perform effective feature 587 selection with the proposed ν -SP-SVMs without incurring in 588 any significant degradation in classification performance. In 589 particular, Table III shows a 25% model complexity reduction 590 in *Image*, Spam, and Wdbc when ν -SP-SVM, as opposed to 591 its standard counterpart, is used. This percentage is even better 592 for other problems, reaching 33.3% in Abalone and Hand and 593 50% in Ionosphere. 594

When we compare the proposed ν -SP-SVM approaches 595 with the RFE method, we observe that the automatic feature 596 selection carried out by our proposals is competitive with stan-597 dard feature selection procedures which have to, first, select 598 the feature subset and, second, train the classifier. According to 599 Table III, results are quite similar for most problems. However, 600

2 AND 1-NORM V-31-5 VIIS IN THE BINAKT CLASSIFICATION I ROBLEMS							
		Standar	d SVM	Dr-SVM	RFE	v-SP	-SVM
			1-norm	DI-3 V IVI	KI L	2-norm	1-norm
Abalone	CE	21.10(±0.89)	20.51(±0.11)	20.60(±0.14)	20.90(±0.58)	20.90(±0.37)	20.85(±0.34)
Abuione	# feat.	8.00(±0.00)	7.96(±0.20)	8.00(±0.00)	4.34(±2.18)	5.36(±2.11)	5.80(±1.87)
Credit	CE	10.65(±0.10)	11.07(±0.13)	11.07(±0.13)	10.99(±0.21)	10.68(±0.15)	11.02(±0.19)
Creati	# feat.	15.00(±0.00)	1.16(±0.55)	2.08(±3.36)	4.32(±4.83)	7.16(±3.15)	1.36(±0.78)
Hand	CE	9.17(±0.18)	9.24(±0.10)	9.20(±0.12)	9.43(±0.22)	9.15(±0.22)	9.29(±0.21)
Папа	# feat.	62.00(±0.00)	55.68(±4.20)	55.56(±4.08)	34.82(±6.04)	45.72(±4.96)	42.06(±5.67)
Image	CE	14.94(±0.95)	12.94(±0.18)	13.11(±0.23)	14.05(±1.07)	13.18(±0.43)	12.98(±0.19)
Image	# feat.	18.00(±0.00)	13.96(±0.20)	17.24(±0.77)	16.06(±1.49)	14.38(±2.58)	13.52(±1.03)
Ionosphere	CE	11.93(±2.02)	11.73(±2.35)	12.38(±0.85)	13.76(±2.12)	11.79(±1.92)	12.27(±1.08)
Tonosphere	# feat.	33.00(±0.00)	24.42(±7.47)	30.92(±3.29)	13.96(±5.13)	18.32(±6.55)	17.44(±3.90)
Pima	CE	23.63(±0.71)	23.29(±0.22)	23.35(±0.31)	23.78(±1.03)	23.36(±0.33)	23.00(±0.20)
1 tma	# feat.	8.00(±0.00)	7.44(±0.50)	7.76(±0.43)	5.26(±2.04)	6.34(±1.14)	6.72(±1.05)
Spam	CE	6.88(±0.17)	7.15(±0.09)	7.03(±0.06)	6.78(±0.21)	6.99(±0.24)	7.09(±0.15)
Span	# feat.	57.00(±0.00)	54.52(±1.79)	56.22(±0.79)	44.68(±3.03)	44.88(±3.21)	42.88(±3.28)
Wdbc	CE	2.97(±0.92)	4.31(±0.68)	3.19(±0.51)	3.43(±0.57)	3.28(±0.53)	3.77(±0.75)
w ubc	# feat.	30.00(±0.00)	18.52(±3.25)	27.38(±3.17)	21.80(±3.59)	22.64(±2.27)	13.80(±2.70)

TABLE III CE AND NUMBER OF SELECTED FEATURES PROVIDED BY STANDARD 2 AND 1-NORM SVMS, DR-SVM, THE RFE METHOD AND THE 2 AND 1-NORM V-SP-SVMS IN THE BINARY CLASSIFICATION PROBLEMS

in the case of *Image*, both v-SP-SVM proposals outperform the 601 RFE method, and for Credit and Wdbc, the 1-norm v-SP-SVM 602 approach achieves the best accuracy-complexity trade-off. On 603 the other hand, in problems such as Ionosphere or Hand, RFE 604 presents a lower number of features, although this advantage 605 is achieved at the expense of a CE increase. 606

Figs. 2 and 3 show the evolution of the classification 607 error and the number of selected features as a function of 608 ν in the different data sets. A dashed line depicts the CE 609 achieved by new standard SVMs retrained with the set of 610 features selected by the proposed v-SP-SVM models and a 611 dotted vertical line points out the ν value selected in the 612 validation process. These figures remark the clear trade-off 613 between the model complexity and the final CE. In problems 614 such as Credit, Image, Ionosphere, and Wdbc, when the 615 1-norm ν -SP-SVM is applied, we could directly have fixed 616 $\nu = 1$, and most useless features would have been removed. 617 However, an adequate selection of v is crucial to obtain an 618 accurate solution. The validation process has carried out a 619 conservative selection of parameter ν , if, during the validation 620 process, a slight performance degradation had been allowed, a 621 additional features would have been removed, in fact, for all 622 the problems under study but *Credit*, lower values of v would 623 have resulted in a lower number of features, while keeping 624 similar error rates. Finally, it is important to note that the 625 retraining procedure does not show any clear improvement, 626 since although in some cases the final CE is slightly improved, 627 in other cases it is similar or, even, slightly worse. 628

C. High Dimensional Datasets 629

The aim of this section is to test the performance of the 630 proposed methods when we are dealing with a large number 631 of input features. For this purpose, the Dexter dataset [40] 632

has been considered. The goal of this problem is to classify 633 texts about "corporate acquisitions" into two categories. The 634 data set has 20000 features, from which 9947 variables 635 correspond to a "bag-of-words" representation of several texts 636 and the remaining 10 053 features are noisy features added 637 to complicate the classification task. The different data set 638 partitions are balanced with 300 training data, 300 validation 639 patterns and 2000 test samples. 640

Due to the large number of input features, the CV of all possible ν values in the ν -SP-SVM methods is not reasonable. For this reason, we have followed this strategy.

- 1) We have first trained the proposed methods with $\nu = 1$, 644 what provides a first approximation to the number of useful features. In this case, 1-norm ν -SP-SVM achieves 646 a CE = 8.1% with only 150 features and 2-norm v-SP-SVM a CE = 6% with 3976 variables.
- 2) According to above number of selected features, the 649 maximum value of ν , worthy of being explored, has been 650 fixed. For instance, in 1-norm ν -SP-SVM this value has 651 been fixed to 0.01 (150 is less than the 1% of 20 000) 652 and in 2-norm ν -SP-SVM has been set to 0.2 (3976 is 653 close to the 20% of 20 000). 654
- 3) Then, a range of 10 linearly spaced ν values has been defined. In particular, ranges $\{0.1\%, 0.2\%, \ldots, 1\%\}$ and $\{2\%, 4\%, \ldots, 20\%\}$ have been explored by each v-SP-SVM model.
- 4) Finally, the optimum ν value has been selected as the one with minimum validation error.

As a result of this procedure, 1-norm ν -SP-SVM has selected 661 a v value of 0.004, achieving a CE = 7.75% with only 662 79 features, whereas 2-norm ν -SP-SVM has used a final ν 663 value of 0.1 providing a CE of 6.4% with 1487 features. 664 Reference methods, 2-norm, 1-norm, and Dr-SVMs, have 665

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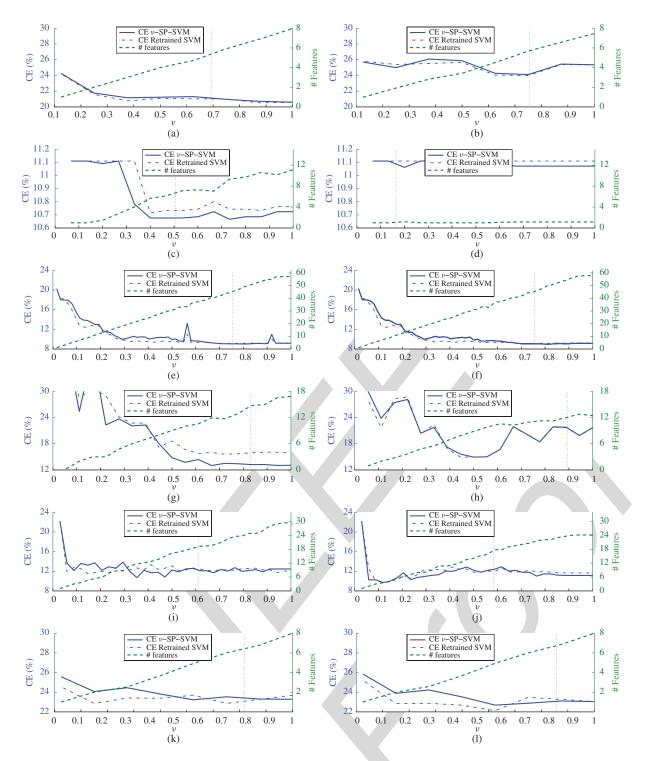


Fig. 2. Evolution of CE and the number of selected features in v-SP-SVMs as a function of v for data sets: *Abalone, Credit, Hand, Image Ionosphere*, and *Pima*. Dash-dotted line shows the CE of an SVM which has been retrained with the features selected by v-SP-SVM model. Dotted vertical line marks the cross-validated v value. (a) 2-norm v-SP-SVM *Abalone*. (b) 1-norm v-SP-SVM *Abalone*. (c) 2-norm v-SP-SVM *Credit*. (d) 1-norm v-SP-SVM *Credit*. (e) 2-norm v-SP-SVM *Hand*. (g) 2-norm v-SP-SVM *Image*. (h) 1-norm v-SP-SVM *Image*. (i) 2-norm v-SP-SVM *Ionosphere*. (j) 1-norm v-SP-SVM *Ionosphere*. (k) 2-norm v-SP-SVM *Pima*. (l) 1-norm v-SP-SVM *Pima*.

presented *CEs* of 6.45%, 8.10% and 6.05%, respectively, and they have used 7142, 159, and 5750 features (see Table IV). These results show that 1-norm ν -SP-SVM outperforms standard 1-norm SVM by achieving a lower *CE* with half the number of features. Regarding 2-norm ν -SP-SVM and standard 2-norm SVM, they present similar error rates, but the latter is using 35% of the features instead of 7.43% used by 2-norm ν -SP-SVM. Finally, Dr-SVM provides the lowest *CE*, but the number of selected features (5750) is much higher than the 1487 of the 2-norm ν -SP-SVM.

Besides, it is important to point out that 1-norm-based algorithms (standard 1-norm SVM and 1-norm ν -SP-SVM) 677

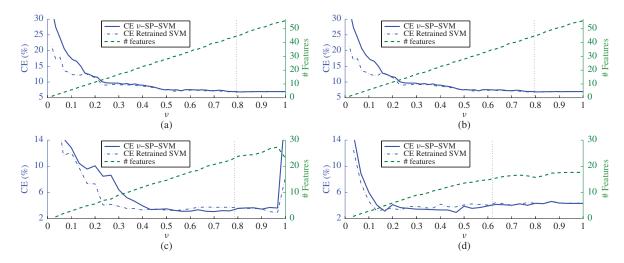


Fig. 3. Evolution of CE and the number of selected features in v-SP-SVMs as a function of v for data sets: *Spam* and *Wdbc*. Dash-dotted line shows the CE of an SVM which has been retrained with the features selected by v-SP-SVM model. Dotted vertical line marks the cross-validated v value. (a) 2-norm v-SP-SVM *Spam*. (b) 1-norm v-SP-SVM *Spam*. (c) 2-norm v-SP-SVM *Wdbc*. (d) 1-norm v-SP-SVM *Wdbc*.

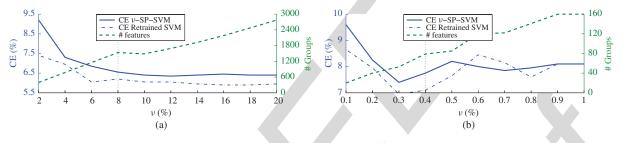


Fig. 4. CE and the number of selected features in ν -SP-SVM algorithms as a function of ν in *Dexter* data set. Dash-dotted line shows the CE of an SVM which has been retrained with the features selected by ν -SP-SVM model. Dotted vertical line marks the cross-validated ν value. (a) 2-norm ν -SP-SVM. (b) 1-norm ν -SP-SVM.

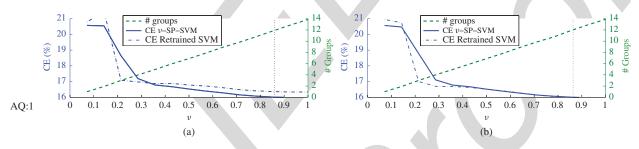


Fig. 5. Evolution of CE and the number of selected features in v-SP-SVMs as a function of v for data sets: *Spam* and *Wdbc*. Dash-dotted line shows the CE of an SVM which has been retrained with the features selected by v-SP-SVM model. Dotted vertical line marks the cross-validated v value. (a) 2-norm v-SP-SVM *Spam*. (b) 1-norm v-SP-SVM *Spam*. (c) 2-norm v-SP-SVM *Wdbc*. (d) 1-norm v-SP-SVM *Wdbc*.

have selected a few number of features, prompting a performance degradation. This effect is due to the fact that the
maximum number of features that can be selected is always
upper bounded by the number of training data [30], [32]. For
this reason, these approaches are working with few hundreds
of features instead of selecting thousands as the 2-norm-based
methods.

Finally, Fig. 4 shows the evolution of the *CE* and the number of features in the model for the explored range of ν values. At first glance, it can be seen that, in the explored range of ν , values larger than 8% in 2-norm ν SP-SVM and 0.3% for 1-norm ν SP-SVM are able to provide accurate results with a low number of features, even lower than 1-norm, 2-norm, and Dr-SVM methods. This figure also shows the *CE* achieved

TABLE IV CE and Number of Selected Features Provided by Different Methods Under Study in Dexter Data Sets

			Standard SVM		v-SP-SVM	
		2-norm	1-norm	Dr-SVM	2-norm	1-norm
Dexter	CE	6.45	8.10	6.05	6.4	7.75
Desier	# feat.	7142	159	5750	1487	79

when the SVM is retrained with the selected set of features, 692 suggesting that, in problems where the number of removed features is high, the retraining process is able to provide an additional advantage in terms of *CE* reduction. 692

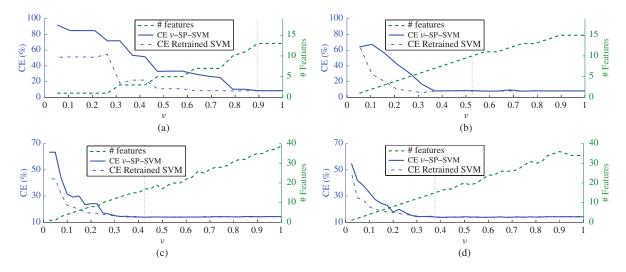


Fig. 6. Evolution of the CE and the number of selected features in ν -SP-SVM algorithms as a function of ν in multiclass problems. Dash-dotted line shows the CE of an SVM which has been retrained with the features selected by ν -SP-SVM model and dotted vertical line marks the cross-validated ν value. (a) 2-norm ν -SP-SVM *Segmentation*. (b) 1-norm ν -SP-SVM *Segmentation*. (c) 2-norm ν -SP-SVM *Wave*. (d) 1-norm ν -SP-SVM *Wave*.

TABLE V PREDEFINED FEATURE GROUPS IN THE PROBLEM ADULT. CATEGORICAL FEATURES ARE CODIFIED WITH DUMMY VARIABLES

# group	Original feature	Categorical / continous	# of categories	# of features in each group
1	age	continuous	-	1
2	workclass	categorical	8	3
3	fnlwgt	continuous	-	1
4	education	categorical	16	4
5	education-num	continuous	-	1
6	marital-status	categorical	7	3
7	occupation	categorical	14	4
8	relationship	categorical	6	3
9	race	categorical	5	3
10	sex	categorical	2	1
11	capital-gain	continuous	-	1
12	capital-loss	continuous	-	1
13	hours-per-week	continuous	-	1
14	native-country	categorical	41	6

696 D. Selecting Feature Groups with v-SP-SVM

To analyze the performance of the proposed methods when 697 features need to be selected according to predefined sets, 698 instead of selecting isolated features, we have chosen the 699 dataset Adult from [38]. The aim of this problem is to 700 determine whether a person earns over 50K a year from 701 several demographic characteristics from 14 original features, 702 of which six are continuous and eight are categorical. Each 703 categorical feature has been coded with dummy variables, 704 using N indicatrix variables (0 or 1) to codify their 2^N 705 possible values, in this way, each data is finally represented 706 by 33 features belonging to 14 groups as it is described in 707 Table V. Then, when a group selection approach is applied, the 708 dummy variables representing to the same categorical feature 709 will be either all selected or all removed from the final model. 710 Note that only when all variables from a certain group are 711

removed it is possible to skip the capture of the associated categorical variable.

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This binary data set has 30162 training samples and 15060 714 data to test the model. To train the different SVMs, we have 715 randomly selected a 10% of the original training data set, 716 therefore, 3016 data have been used to train the different meth-717 ods. A 5-fold CV process has been applied to adjust the free 718 parameters of the different methods and their performances 719 have been evaluated over whole test data. The different SVMs 720 have been trained 100 times, with different randomly selected 721 training data, and their averaged results have been studied. 722

As result, standard 2 and 1-norm SVMs present an averaged 723 CE of $16.33(\pm 0.3)\%$ and $15.97(\pm 0.2)\%$ employing 14 and 724 13.9 ± 0.3 groups, respectively, whereas Dr-SVM presents 725 the same performance (both in CE and number of selected 726 features) as 1-norm SVMs. This result is a consequence of 727 standard 2-norm SVM having selected all groups and 1-norm 728 SVM and Dr-SVM having seldom discarded group 10, this 729 group is associated to original feature sex and codified with 730 only one dummy variable. 731

To compare these results with the proposed methods, Fig. 5 732 depicts the values of the CE and the number of selected 733 groups as a function of parameter ν in ν -SP-SVMs. It can 734 be seen that if ν is cross validated (see dotted vertical line), 735 ν -SP-SVMs present CE close to 16% with 12 groups, since 736 groups 3 and 10 are usually removed. However, if we had 737 wanted to select a lower number of groups, v could have 738 been fixed around 0.3, keeping the CE lower than 17% and 739 selecting just the 4 most relevant groups: Groups associated to 740 original features education-num, relationship, and capital-gain 741 are always chosen and additionally, either group 4 (education) 742 or 7 (occupation) is included in the model. Thus, this example 743 illustrates the convenience of the ν formulation of SP-SVM for 744 allowing a more flexible selection of the number of variables 745 to be incorporated in the model. 746

Again, a retraining process (dash-dotted line in Fig. 5) $_{747}$ provides a small improvement, since for most ν values, $_{748}$ ν -SP-SVMs, and retrained SVMs achieve similar CEs. $_{749}$

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		Classica	Classical SVMs		Sparse SVMs	
		2-norm	1-norm	Dr-SVM	2-norm	1-norm
Segmentation	CE	9.05	9.00	8.24	8.43	8.52
Segmentation	# feat.	18.00	13.00	15	13.00	10.00
Wave	CE	13.87	14.33	14.20	13.87	14.07
wave	# feat.	40.00	38.00	30.00	17.00	15.00

TABLE VI CE and Number of Selected Features Provided by Different Methods Under Study in Multiclass Data Sets

750 E. Multiclass Problems

In this section, we will test the performance of the 751 v-SP-SVMs over multiclass datasets Segmentation and Wave 752 from the UCI repository [38]. The purpose of Segmentation 753 problem is to classify hand-segmented images represented by 754 19 features in 7 categories: brickface, sky, foliage, cement, 755 window, path, and grass. The data set has 210 and 2100 756 training and test data, respectively. Wave problem consists of 757 3 classes of waves to be identified from 40 features, whose 758 latter 19 ones are all noise, the data set has 3500 training 759 samples and 1500 test data. As in the previous sections, the 760 free parameters of the different methods have been adjusted 761 with a 5 fold CV process. 762

To train the different classifiers, proposed ν -SP-SVM meth-763 ods have solved problem (10), either in its 2-norm or in its 764 1-norm version, whereas reference methods have directly used 765 the multiclass problem defined by (9) with their corresponding 766 penalization terms. Table VI presents the results achieved by 767 both standard and proposed SVMs. As it can be observed, 768 ν -SP-SVMs achieve lower error rates with lower number of 769 features. In Segmentation, CE is reduced in a 0.5%, with 770 respect to 1-norm and 2-norm SVMs, using only 13 and 771 10 features, whereas Dr-SVM achieves a slightly lower CE 772 using 15 features. In Wave, the advantages of the proposed 773 SVM classifiers are clearer, since the number of features in 774 the model is half the number for the reference methods and 775 the CE is similar in the 2-norm models, slightly reduced in 776 the 1-norm methods and Dr-SVMs are outperformed by both 777 v-SP-SVMs. 778

⁷⁷⁹ When the evolution of CE and the number of features are ⁷⁸⁰ analyzed as a function of ν (see Fig. 6), the trade-off between ⁷⁸¹ these parameters is again observed. Besides, retrained SVMs ⁷⁸² provide a significant CE reduction in *Segmentation* problem.

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V. CONCLUSION

This paper introduced a method for feature selection based 784 on a new formulation of linear SVMs that includes constraints 785 additional to the classical ones. These constraints drop the 786 weights associated to those features that are likely to be 787 irrelevant. In order to predefine an upper bound for the number 788 of relevant features, a v-SVM formulation has been used, 789 where ν is a parameter that indicates the fraction of features 790 to be considered. This parameter is swept in an efficient 791 way in order to find the optimal number of features over 792 a validation set of data. This paper presented two versions 793

of the formulation, the first one being an SVM with a 2-794 norm regularization term. The second one uses a 1-norm 795 regularization, that has a reduced computational burden with 796 respect to the first one. Besides, this new SVM formulation 797 allows us to easily apply the feature selection process over 798 predefined feature sets. This, in turn, is useful to introduce a 799 straightforward, yet efficient way to extend the algorithms to 800 multiclass problems. 801

Experiments showed that the introduced methods present advantages not only in terms of CE, but also in the ability of reducing the model complexity by adequately removing features during the training process, not as a preprocessing stage. Also, these experiments showed that the algorithms are efficient when applied to the task of feature group selection and to multiclass problems.

Future research includes nonlinear versions of the algorithm in order to take into account the nonlinear relationships between features. Applications can also include extensions to regression problems as well as linear model selection for signal processing tasks, such as filter design or plant modeling, in situations where optimal models are known to be sparse.

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Support Vector Machines with Constraints for Sparsity in the Primal Parameters

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Abstract—This paper introduces a new support vector 1 machine (SVM) formulation to obtain sparse solutions in the 2 primal SVM parameters, providing a new method for feature 3 selection based on SVMs. This new approach includes additional 4 constraints to the classical ones that drop the weights associated 5 to those features that are likely to be irrelevant. A v-SVM 6 formulation has been used, where ν indicates the fraction of features to be considered. This paper presents two versions of 8 the proposed sparse classifier, a 2-norm SVM and a 1-norm SVM, 9 the latter having a reduced computational burden with respect to 10 the first one. Additionally, an explanation is provided about how 11 12 the presented approach can be readily extended to multiclass classification or to problems where groups of features, rather 13 than isolated features, need to be selected. The algorithms have 14 been tested in a variety of synthetic and real data sets and they 15 have been compared against other state of the art SVM-based 16 linear feature selection methods, such as 1-norm SVM and doubly 17 regularized SVM. The results show the good feature selection 18 ability of the approaches. 19

Index Terms—Feature group selection, feature selection,
 margin maximization, multiclass classification, support vector
 machines.

I. INTRODUCTION

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UPPORT vector machines (SVMs) [1], [2] are considered 24 the state-of-art in machine learning due to their well 25 known good performance in a wide range of applications 26 [3]-[5]. The SVM criterion minimizes a loss term, called hinge 27 loss, plus an additional quadratic penalization term which 28 regularizes the solution [6]. This hinge loss minimization 29 allows SVMs to approximate Bayes' rule without estimating 30 the conditional class probability [7] and makes it converge to 31 a maximum margin solution [8], thus endowing SVMs with 32 good generalization properties. 33

In spite of the generally good performance of SVMs, in many practical situations, useless, redundant, or noisy features can degrade the attained solution. The reason for this is that

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the SVM solution is based on a combination of all input features, including the irrelevant ones. As it is stated in the bet-on-sparsity principle [9], this situation is undesired and it would be preferable to obtain a solution consisting only of the relevant features. That way, more accurate and interpretable solutions can be achieved.

To achieve this goal, a feature selection process [10], [11] is 43 usually applied. Classical feature selection techniques, such as 44 filtering [12] or wrapping [13], [14] approaches, are used as an 45 independent preprocessing step before the training of the final 46 classification (or regression) machine. More recent feature 47 selection methods combine the feature selection process with 48 the final predictor training. For instance, in [15]-[17] an 49 objective function that combines an accuracy prediction term 50 with a term associated to the sparsity in the number of selected 51 variables is employed. In [18]–[20] the SVM prediction output 52 is considered as a linear combination of kernel functions and 53 then, the prediction accuracy is evaluated as a function of the 54 used and discarded features. This method, known as recursive 55 feature elimination (RFE), has been widely employed for SVM 56 classification, however, recent works [21] have shown that 57 RFE is not consistent with maximum margin solutions. 58

In contrast to the approaches that include an explicit feature selection strategy (either independent or combined with the classification step), classifiers directly providing sparse solutions are usually preferred. Following this point of view, the LASSO method was proposed in [15]. LASSO includes a 1-norm regularization term in the optimization problem. Since this norm has a singularity at the origin, some coefficients of the solution vector are shrunk to zero, what provides sparse solutions. Since then, many researchers have focused their work on minimizing 1-norm penalized functions [22]–[24]. In fact [25] points out the need and usefulness of linear sparse solutions in problems like functional magnetic resonance imaging.

In [26], the classical SVM formulation is modified by replacing the quadratic penalization term with a 1-norm penalty, what leads to solutions with sparse coefficients. Although this SVM formulation can only be used for feature selection in linear classification problems, this approach has nevertheless been successfully used in a large number of applications, such as computational biology [27], [28], drug-design [17] or gene microarrays classification [29], among others.

Although 1-norm SVMs retain most of the desired properties of classical SVMs, such as margin maximization, they may fail to provide good solutions in certain situations. As it is

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usually outperform their 1-norm counterparts. Furthermore, as 85 it is pointed out in [30] and [31], the 1-norm SVM presents two 86 additional limitations: first, when there are highly correlated 87 variables, it usually removes some of them, and, second, the 88 maximum number of selected features is limited by the number 89 of available training data. Trying to overcome these draw-90 backs, elastic nets [32] and their particularization to SVMs 91 by means of the doubly regularized support vector machine 92 (Dr-SVM) [30], [31] are proposed, this new approach gener-93 alizes the LASSO and 1-norm SVM methods by keeping the 94 2-norm regularization term and including an additional 1-norm 95 penalty term to force sparsity. Despite common improved 96 performance of Dr-SVM, both 1-norm and Dr-SVMs are not 97 suitable methods when the underlying model is truly sparse, 98 since they are not able to remove all unnecessary variables 99 from the final classifier, this problem was already remarked 100 for 1-norm SVMs in [33] and, in the experimental section of 101 this paper, we will illustrate it for Dr-SVM. 102

An additional limitation of 1-norm SVM and Dr-SVM, is 103 that they are not well suited to multiclass classification or 104 to problems where features have to be selected or removed 105 using predefined groups. One possible solution could consist 106 in adding a group LASSO [34] or an ∞ -norm [35] penaliza-107 tion term into the SVM formulation. However, both options 108 result in a more complex SVM formulation, which cannot be 109 solved with standard linear programming (LP) or quadratic 110 programming (QP) solvers. 111

In this paper, a new SVM formulation for the linear case 112 is presented that directly forces sparse solutions. Rather than 113 modifying the objective function, additional constraints are 114 included in the minimization task in order to identify irrelevant 115 features and to drop their associated weights to values lower 116 than a small parameter ε . This constant can be adjusted during 117 the optimization problem resolution by predefining the number 118 of relevant features to be kept in the final solution using a 119 ν -SVM formulation [36]. We will show that these additional 120 constraints can be incorporated to force sparsity in both 121 2-norm and 1-norm SVM formulations. Our approach allows 122 to overcome the limitations of 1-norm SVMs and Dr-SVMs 123 in different ways. First, by properly adjusting parameter ν , 124 the algorithm is able to remove all irrelevant features from 125 the final model. Second, the proposed formulation can be 126 applied to the selection of isolated features or predefined 127 feature groups where needed. Finally, as it will be shown in 128 the experiments section, more accurate solutions are usually 129 achieved, particularly, when using the new constraints together 130 with the 2-norm SVM. 131

The rest of this paper is organized as follows. In the next 132 section, we introduce our approach to force feature selection 133 in SVM classifiers, explaining how it can be applied both to 134 2-norm and 1-norm formulations. Section III presents some 135 extensions of the method to address the selection of features 136 in predefined groups of variables, as well as for multiclass 137 classification problems. Section IV presents extensive simu-138 lation work to illustrate the performance of our approach, 139 and its advantages with respect to previous proposals for 140

feature selection in SVMs. Finally, Section V presents the 141 main conclusion of our work, and identifies some lines for 142

II. SVM WITH EXPLICIT CONSTRAINTS FOR 144 FEATURE SELECTION

A. Problem Overview

In this paper, we consider classification problems where 147 the representation of the input data contains some features, 148 which are irrelevant for the task at hand. This may happen 149 as a consequence of redundancy between the input variables 150 or, simply, because some of the input features do not carry 151 any valuable information for the classification. In a standard 152 machine learning setup, we are given a set of N training 153 labeled data, $S = {\mathbf{x}^{(l)}, y^{(l)}}, l = 1, \dots, N$, where $\mathbf{x}^{(l)} \in$ 154 \Re^d are the input vectors and $y^{(l)}$ are used to encode class 155 membership, from which we have to learn both the subset of 156 relevant input variables and the classification function itself. 157

Linear classifiers obtain their outputs according to a thresh-158 olded version of the estimator 159

$$\hat{\mathbf{y}} = \mathbf{w}^T \mathbf{x} + b \tag{1}$$
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where \hat{y} is the output of the classifier for input vector **x**, 161 \mathbf{w} is the vector that defines the classifier, and b is a bias 162 term. For the SVM case, the Representer's Theorem [1], [2] 163 states that the solution vector will lie in the subspace spanned 164 by all training vectors $\{\mathbf{x}^{(l)}\}$. When irrelevant features are 165 present in the data we can carry out a pre-processing stage to 166 select the most informative variables or, alternatively, discard 167 the variables x_i whose associated weight w_i is exactly zero 168 after the optimization of the classifier. However, since noise is 169 normally present in the data, none of the components of w will 170 be exactly zero unless sparsity is included as an optimization 171 criterion during the training of the classifier. 172

A standard way to impose sparsity in w is to include 173 a regularization term in the cost function, based on the 174 1-norm of **w**, i.e., $\|\mathbf{w}\|_1 = \sum_i |w_i|$. This regularizer presents 175 singularity points whenever any of the components of w is 176 zero, what tends to nullify some of the solution weights, thus 177 favoring sparse solutions. However, this mechanism does not 178 necessarily imply that all weight components associated to 179 irrelevant variables will become zero [33]. 180

Rather than modifying the structural risk term in the SVM 181 functional, in this paper, we propose a new approach to impose 182 sparsity in the solution by introducing a set of additional 183 constraints for the optimization problem. We will see that 184 our method is able to automatically identify all irrelevant 185 features, thus constituting an effective mechanism for imple-186 menting SVMs that incorporate a feature selection approach. 187 Furthermore, since the 2-norm regularization term can still be 188 used, this usually results in a better performance when the true 189 underlying solution is non sparse. 190

B. 2-Norm SVMs with Sparsity Constraints

Classical SVMs are based on the minimization of a func-192 tional that includes two terms. The first term is the squared 193 norm of the weight vector \mathbf{w} , which is inversely proportional 194

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to the margin of classification [1], thus, this term is related
to the structural risk of the classifier and to its generalization
capabilities. The second term in the objective functional, which
is known as the empirical risk term, is a sum of errors over
the training data. In other words, the linear SVM problem can
be stated as

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min
$$\|\mathbf{w}\|^{2} + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)}$$

s.t. $y^{(l)} (\mathbf{w}^{T} \mathbf{x}^{(l)} + b) \ge 1 - \xi^{(l)}; \quad \forall l$
 $\xi^{(l)} \ge 0; \quad \forall l$ (2)

where slack variables $\xi^{(l)}$ are introduced to allow some of the training patterns to be misclassified or to lie inside the classifier margin, and where *C* is a constant that controls the trade-off between the structural and empirical risk terms.

As it is well known, this optimization method provides a sparse solution in the sense that **w** is a linear combination of only a subset of the training data [the so-called support vectors (SVs)]. However, if feature selection is pursued during the optimization, a solution sparse in the parameters **w** is needed. In order to obtain such a solution, we will introduce some additional constraints in the optimization problem.

We start by rewriting each of the weight components, 213 $w_i, i = 1, \dots, d$, as $w_i = u_i - v_i$, with $u_i, v_i \ge 0$. As 214 we will explain later, our optimization problem will implicitly 215 enforce that at least one of the two terms in the subtraction, 216 u_i or v_i , is zero, depending on whether the optimal weight is 217 positive $(u_i > 0 \text{ and } v_i = 0)$, negative $(u_i = 0 \text{ and } v_i > 0)$ or 218 zero $(u_i = v_i = 0)$. Therefore, the square norm of the weight 219 vector is given, in terms of these new variables, by 220

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$$\|\mathbf{w}\|_{2}^{2} = \sum_{i=1}^{d} u_{i}^{2} + v_{i}^{2}.$$
 (3)

Furthermore, in order to obtain a sparse solution in w, we introduce some additional constraints to upper bound the absolute value of weight components by a small constant ε , i.e., $|w_i| = u_i + v_i < \varepsilon$. Introducing (3) and the new constraints into (2), we get the following modified SVM formulation:

$$\min \sum_{i=1}^{d} (u_i^2 + v_i^2) + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)} + \frac{C'}{d} \sum_{i=1}^{d} \gamma_i$$
s.t. $y^{(l)} \left[\sum_{i=1}^{d} (u_i - v_i) x_i^{(l)} + b \right] \ge 1 - \xi^{(l)}; \quad \forall l$
 $\xi^{(l)} \ge 0; \quad \forall l$
 $u_i + v_i \le \varepsilon + \gamma_i; \quad \forall i$
 $u_i, v_i \ge 0; \quad \forall i$
 $\gamma_i \ge 0; \quad \forall i.$

$$(4)$$

Although the above optimization problem has not explicitly included, the constraint $u_i v_i = 0$, (4) is indirectly forcing that either u_i or v_i is equal to 0. Note that among all possible pairs of values (u_i, v_i) that are able to provide a certain value w_i , the pair which minimizes $\sum_{i=1}^{d} (u_i^2 + v_i^2)$ has to fix either u_i or v_i to 0, for instance, for positive w_i and according to its definition in terms of u_i and v_i , minimization of the functional in (4) will lead to $v_i = 0$ and $u_i = w_i$. The opposite situation will occur for $w_i < 0$.

Note that in our redefinition of the problem we have 237 introduced new slack variables γ_i and those slack variables 238 associated with relevant features will be greater than zero after 239 the functional optimization. Thus, these constants need to be 240 introduced in the objective functional weighted with a trade-241 off parameter C'. The above minimization problem can be 242 directly solved in the primal over the variables u_i , v_i , b, γ_i , 243 and $\xi^{(l)}$, using standard QP algorithm. 244

We can now get some insight into the sparsity mechanism 245 that has been adopted. If irrelevant features are present in the 246 input representation space, most classification schemes would 247 still assign them a non zero weight w_i due to the noise present 248 in the data. However, if a w_i value greater than ε were assigned 249 in our scheme, γ_i would be strictly positive, increasing the 250 value of the functional. Thus, on the one hand irrelevant 251 features that do not significantly decrease the empirical error 252 term will simply be assigned weights smaller, in absolute 253 terms, than ε . On the other hand, components w_i which are 254 necessary to define the SVM solution will have values larger 255 than ε . It is straightforward to use the values of slacks γ_i after 256 the optimization to check whether a variable has been removed 257 or incorporated into the classification model. 258

This new SVM with sparsity constraints performs feature 259 selection on the input variables, so we will hereafter refer to 260 it as sparse primal support vector machine (SP-SVM). 261

At first sight, one could think that the sparsity constraints in 262 (4) are equivalent to a 1-norm penalty term and thus algorithm 263 (4) is equivalent to Dr-SVM. Nevertheless, these constraints 264 have been introduced here through an ε -insensitive cost func-265 tion. As we will analyze along this paper, this new formulation 266 provides two advantages: 1) the sparsity of the model can be 267 easily adjusted by the user through a v SVM formulation, 268 and 2) extensions of this model to group feature selection and 269 multiclass problems are straightforwardly derived. 270

The computational cost of (4) is larger than that of 271 1-norm or Dr-SVMs due to the new constrains. However, an 272 efficient implementation of the problem, which exploits the 273 sparse formulation of these constrains, it results in a very 274 moderate computational increase. 275

Finally, it is important to point out that a major limitation of problem (4), as well as 1-norm and Dr-SVM algorithms, is their linear formulation. Note that their non linear extension would provide a non linear boundary with a kernel selection mechanism, instead of an automatic feature selection criterion.

C. 2-Norm v-SP-SVM

In this section, we introduce a modification of the SP-SVM formulation in (4) to automatically adjust the value of ε , following the ν -SVM that was introduced in [36]. In this formulation of the SVM, ε is traded off against model complexity and slack variables through a constant $\nu \in (0, 1]$. Then, the optimization problem to solve is given by 287

$$\min \quad \sum_{i=1}^{d} (u_i^2 + v_i^2) + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)} + C' \left[v\varepsilon + \frac{1}{d} \sum_{i=1}^{d} \gamma_i \right] \qquad _{288}$$

s.t.
$$y^{(l)} \left[\sum_{i=1}^{d} (u_i - v_i) x_i^{(l)} + b \right] \ge 1 - \xi^{(l)}; \quad \forall l$$

$$\xi^{(l)} \ge 0; \quad \forall l$$

$$u_i + v_i \le \varepsilon + \gamma_i; \quad \forall i$$

$$u_i, v_i \ge 0; \quad \forall i$$

$$\gamma_i \ge 0; \quad \forall i$$

$$\varepsilon \ge 0.$$

(5)

As above, this optimization problem can be directly solved in 290 the primal, with respect to variables u_i , v_i , b, γ_i , $\xi^{(l)}$, and ε . 291 It is well known [36] that, when the standard ν support 292 vector regression is applied resulting a non zero ε , ν is an 293 upper bound on the fraction of errors and a lower bound on 294 the fraction of SVs. Note that in (5), if the dual formulation of 295 the problem was used and we let $\{\beta_i\}_{i=1}^d$ be the dual variables 296 associated to the sparsity constraints, the following equalities 297 had to be verified: 298

 $\sum_{i=1}^{d} \beta_i \le \frac{C'}{d} \nu$

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$$0 \le \beta_i \le \frac{C'}{d}$$

what forces v to be an upper bound of the number of dual 301 variables β_i taking a value of C'/d, that is, ν is an upper 302 bound over the number of slack variables γ_i different from 0. 303 This leads to a useful result for the proposed ν -SP-SVM: ν 304 is an upper bound on the fraction of components of \mathbf{w} whose 305 absolute value is less than ε . In other words, parameter ν can 306 be used to control the sparsity of the solution, setting a priori 307 the maximum number of features that can be selected by the 308 2-norm v-SP-SVM. 309

310 D. 1-Norm v-SP-SVM

Using the 1-norm of w in the structural risk term of 311 classical SVMs leads to LP problems, which have a reduced 312 computational burden when compared to the QP formulation 313 required for 2-norm SVMs. Similar benefits can be obtained 314 for the SP-SVM proposed in the previous sections. Note that 315 the constraints that were imposed in order to force sparsity 316 do not affect the regularizer for w in any way, thus, in order 317 to extend either (4) or (5) to the 1-norm case, it is sufficient 318 to replace the structural risk term accordingly. For instance, 319 for the ν -SP-SVM in its 1-norm version this leads to 320

$$\min \sum_{i=1}^{d} (u_i + v_i) + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)} + C' \left[v\varepsilon + \frac{1}{d} \sum_{i=1}^{d} \gamma_i \right]$$

s.t.
$$y^{(l)} \left[\sum_{i=1}^{d} (u_i - v_i) x_i^{(l)} + b \right] \ge 1 - \xi^{(l)}; \quad \forall l$$
$$\xi^{(l)} \ge 0; \quad \forall l$$
$$u_i + v_i \le \varepsilon + \gamma_i; \quad \forall i$$
$$u_i, v_i \ge 0; \quad \forall i$$
$$\gamma_i \ge 0; \quad \forall i$$
$$\varepsilon > 0.$$
 (6)

Using LP optimization tools, this problem can be solved in a more efficient way than with QP optimizers, obtaining the values of u_i , v_i , and b that define the solution. As with the 2-norm formulation, the selected features will be those whose corresponding slacks γ_i are greater than zero.

III. SP-SVM EXTENSIONS

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In this section, we consider two different extensions of 328 our SVM with feature selection. First, we will consider the 329 joint selection (or removal) of features that are assigned to 330 predefined groups, second, we will study how the SP-SVM can 331 be extended to multi-class problems. During our derivations in 332 this section, we will only consider the ν -SP-SVM formulation 333 with 2-norm for the regularization term, although it would 334 be straightforward to apply similar extensions to the standard 335 SP-SVM or 1-norm v-SP-SVM. 336

A. v-SP-SVM with Feature Selection Over Predefined Groups 337

In some practical situations, variables can appear grouped 338 together in predefined sets that can be jointly relevant or 339 irrelevant. Then, the feature selection process must be applied 340 over these sets rather than over the isolated features. This 341 is for instance the case when encoding categorical variables 342 with binary words. Either all binary variables corresponding 343 to the same categorical feature should be selected or removed 344 together. 345

Let us assume that the input features are structured in G < d346 disjoint groups, i.e., each input feature belongs to exactly 347 one group. Let us also denote by S_g the indexes of the g-th 348 group of variables, with $g = 1, \ldots, G$. Then, we can modify 349 (5) by replacing the constraints over the absolute values of 350 each individual weight (i.e., $u_i + v_i \le \varepsilon + \gamma_i$) by alternative 351 constraints each one consisting of the sum of absolute values 352 of all weights corresponding to the variables belonging to the 353 same group 354

$$\min \sum_{i=1}^{d} (u_i^2 + v_i^2) + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)} + C' \left[v\varepsilon + \frac{1}{G} \sum_{g=1}^{G} \gamma_g \right]$$
s.t.
$$y^{(l)} \left[\sum_{i=1}^{d} (u_i - v_i) x_i^{(l)} + b \right] \ge 1 - \xi^{(l)}; \quad \forall l$$

$$\xi^{(l)} \ge 0; \quad \forall l \qquad (7) \quad {}_{355}$$

$$\sum_{i \in S_g} u_i + v_i \le \varepsilon + \gamma_g; \quad \forall g$$

$$u_i, v_i \ge 0; \quad \forall i$$

$$\gamma_g \ge 0; \quad \forall g$$

$$\varepsilon > 0$$

where γ_g are slacks associated to each group and γ_g values greater than 0 after optimization indicate, which groups have been selected and included in the classification model. Now, parameter ν can be used to *a priori* establish the maximum number of groups that should be selected by the algorithm, thus providing a control mechanism for adjusting the degree of sparsity desired for the solution.

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Finally, it is important to point out some advantages of this formulation with regard to other reference methods.

- 1) The standard formulation of 1-norm SVMs [26] cannot be used for feature selection in the setup that we have studied here. This is due to the fact that standard 1-norm SVM directly introduces term $||\mathbf{w}||_1$ in the objective function to force sparsity, making it impossible to force all coefficients of the same group to shrink to zero at the same time.
- 2) Forcing sparsity over groups with a group LASSO 372 penalty term [34] precludes the standard SVM formu-373 lation, since it turns it out into a non linear convex 374 optimization problem. Feature selection over groups 375 only implies a modification of the introduced con-376 straints due to the fact that our approach forces spar-377 sity by means of additional constraints; therefore, stan-378 dard LP or QP optimizers can be used to solve the 379 problem. 380
- 3) Furthermore, if 1-norm were used to penalize weights
 coefficients in the functional of (7), not only groups
 selection would be implemented, but also sparsity within
 the groups would be favored.

385 B. Multiclass v-SP-SVM

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Here, we present the extension to multiclass classification problems by following the SVM multiclass approach from [37]. Let us consider a classification problem with *K* classes. Then, in this case we have $y^{(l)} \in \{1, ..., K\}$. Accordingly, the classification function for a linear classifier is given by

$$\hat{y} = \arg \max_{k=1,\dots,K} \mathbf{w}_k^T \mathbf{x} + b_k \tag{8}$$

i.e., *K* different outputs associated to each class are computed, and then the pattern is classified according to the largest output. The set of vectors and bias terms $\{\mathbf{w}_k, b_k\}, k =$ $1, \ldots, K$, which define the classifier can be obtained as the solution to the following optimization problem:

$$\min \sum_{k=1}^{K} \|\mathbf{w}_{k}\|^{2} + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)}$$

s.t. $\left[\mathbf{w}_{y^{(l)}}^{T} \mathbf{x}^{(l)} + b_{y^{(l)}}\right] - \left[\mathbf{w}_{m}^{T} \mathbf{x}^{(l)} + b_{m}\right] \ge 2 - \xi^{(l)};$ (9)
 $\forall l; \ m \neq y^{(l)}$
 $\xi^{(l)} > 0 \quad \forall l.$

As with the binary SVM, the objective function consists of the 399 sum of two terms that are related to the structural and empirical 400 risks. The constraints for the minimization try to force that, 401 for each training sample, the largest output of the system is 402 obtained for the correct class. Otherwise, slack variable $\xi^{(l)}$ 403 will take a value equal to the distance between the largest 404 output and the output associated to the actual class of the 405 pattern [37]. 406

We can now introduce sparsity constraints to allow feature selection during the training of the multiclass SVM. A straightforward extension of our strategy for the binary case would lead to

$$\min \sum_{k=1}^{K} \sum_{i=1}^{d} (u_{k,i}^{2} + v_{k,i}^{2}) + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)} + C' \left[v\varepsilon + \frac{1}{Kd} \sum_{k=1}^{K} \sum_{i=1}^{d} \gamma_{k,i} \right] \text{s.t.} \left[\sum_{i=1}^{d} (u_{y^{(l)},i} - v_{y^{(l)},i}) x_{i}^{(l)} + b_{y^{(l)}} \right] - \left[\sum_{i=1}^{d} (u_{m,i} - v_{m,i}) x_{i}^{(l)} + b_{m} \right] \ge 2 - \xi^{(l)}; \forall l; \ m \neq y^{(l)} \xi^{(l)} \ge 0; \quad \forall l u_{k,i} + v_{k,i} \le \varepsilon + \gamma_{k,i}; \quad \forall i; \ \forall k u_{k,i}, v_{k,i} \ge 0; \quad \forall i; \ \forall k \gamma_{k,i} \ge 0; \quad \forall i; \ \forall k \varepsilon \ge 0$$
 (10)

where we have defined $\mathbf{w}_k = \mathbf{u}_k - \mathbf{v}_k$, and $u_{k,i}$ and $v_{k,i}$ are the *i*-th components of \mathbf{u}_k and \mathbf{v}_k , respectively.

The above formulation would result in vectors \mathbf{w}_k with 414 different sparsity distributions. It should be noted, however, 415 that in order to perform a true feature selection, it would be 416 necessary that the irrelevant features are removed from all 417 \mathbf{w}_k at the same time. In other words, to discard a feature 418 x_i from the final classification model, it is necessary that 419 such a feature is simultaneously ignored for the computation 420 of all K system outputs. In order to do so, we can use an 421 approach similar to that in Section III-A, including in a single 422 constraint all weights $u_{k,i}$ and $v_{k,i}$ associated to the same 423 feature. Proceeding in this way, (10) is changed into 424

$$\min \sum_{k=1}^{K} \sum_{i=1}^{d} (u_{k,i}^{2} + v_{k,i}^{2}) + \frac{C}{N} \sum_{l=1}^{N} \xi^{(l)}$$

$$+ C' \left[v\varepsilon + \frac{1}{d} \sum_{i=1}^{d} \gamma_{i} \right]$$
s.t.
$$\left[\sum_{i=1}^{d} (u_{y^{(l)},i} - v_{y^{(l)},i}) x_{i}^{(l)} + b_{y^{(l)}} \right]$$

$$- \left[\sum_{i=1}^{d} (u_{m,i} - v_{m,i}) x_{i}^{(l)} + b_{m} \right] \ge 2 - \xi^{(l)}; \quad \forall l; \ m \neq y^{(l)}$$

$$\xi^{(l)} \ge 0; \quad \forall l$$

$$\sum_{k=1}^{K} u_{k,i} + v_{k,i} \le \varepsilon + \gamma_{i}; \quad \forall i$$

$$u_{k,i}, v_{k,i} \ge 0; \quad \forall i; \forall k$$

$$\gamma_{i} \ge 0; \quad \forall i$$

$$\varepsilon \ge 0.$$

$$(11)$$

The above problem can be solved using QP optimizers. At the solution, those features with an associated $\gamma_i > 0$ will be selected, while all the rest are excluded from the classifier.

TABLE I

CE RATES AND NUMBER OF FEATURES PROVIDED IN THE ORANGE DATA PROBLEM BY THE DIFFERENT METHODS UNDER STUDY: STANDARD 2 AND 1-NORM SVMS, Dr-SVM and 2 and 1-NORM *v*-SP-SVMS. PARAMETERS *q* and *p* INDICATE THE NUMBER OF RANDOM FEATURES INCLUDED IN THE DATA SET AND THE TOTAL NUMBER OF FEATURES IN THE EXPANDED INPUT SPACE, RESPECTIVELY

a n		Standar	d SVM	Dr-SVM	v-SP-	SVM
<i>q</i> , <i>p</i>		2-norm	1-norm	DI-5 V WI	2-norm	1-norm
0, 5	CE	7.87(±2.15)	7.30(±1.18)	7.30(±1.08)	6.89(±1.08)	6.89(±1.07)
0, 5	# feat.	-	4.46(±0.93)	4.75(±0.63)	2.66(±0.94)	2.67(±0.91)
2, 14	CE	10.56(±2.50)	8.16(±1.18)	8.42(±1.39)	6.78(±1.16)	6.81(±1.15)
2, 14	# feat.	-	6.34(±3.40)	7.46(±3.30)	2.45(±1.28)	2.27(±0.88)
4, 27	CE	13.83(±2.88)	8.71(±1.39)	8.84(±1.60)	6.88(±1.28)	6.91(±1.36)
4, 27	# feat.	-	6.49(±4.65)	9.79(±3.26)	2.48(±1.35)	2.27(±0.87)
6, 44	CE	15.89(±3.01)	8.75(±1.34)	9.19(±1.61)	6.64(±1.23)	6.74(±1.34)
0, 44	# feat.	-	6.41(±4.93)	13.56(±3.79)	2.36(±1.65)	2.44(±1.47)
8, 65	CE	18.81(±2.92)	8.93(±1.49)	10.05(±2.07)	6.76(±1.37)	6.85(±1.47)
0, 05	# feat.	-	6.22(±4.21)	18.63(±5.02)	2.27(±1.21)	2.38(±1.42)
12, 119	CE	23.59(±2.83)	8.80(±1.16)	11.11(±2.94)	6.64(±1.24)	6.70(±1.22)
12, 119	# feat.	-	7.60(±3.04)	25.44(±8.41)	2.15(±1.27)	2.21(±1.32)
16, 189	CE	27.18(±2.65)	8.98(±1.40)	12.86(±3.54)	6.84(±1.30)	6.97(±1.34)
10, 109	# feat.	-	10.00(±4.65)	34.81(±8.49)	2.53(±2.10)	2.56(±1.80)

As before, parameter ν can be used to control the maximum 429 number of features to be selected by the multiclass ν -SP-SVM. 430 Similarly to what we explained for the group selection case, 431 imposing sparsity through additional constraints is key in order 432 to perform a common feature selection for all classification 433 problems, and approaches relying on the introduction of 434 1-norm penalties in the objective function would either fail to 435 select the same features for all classification tasks, or preclude 436 the use of standard LP or QP optimizers. 437

IV. EXPERIMENTS

In this section, we will test the performance of the proposed 2 and 1-norm ν -SP-SVM algorithms. For this purpose, we will analyze both the provided classification error (CE) rate and the number of selected features compared to those of standard 2 and 1-norm SVMs, as well as the Dr-SVM from [30].

In all experiments, free SVM parameters have been opti-444 mized through a cross validation (CV) process. Parameter C445 of standard SVMs has been logarithmically swept with 10 446 values from 10⁻²N to 10⁶N, N being the number of training 447 data. Parameter C of ν -SP-SVMs has been explored with 5 448 values in the same range. For each value of C, C' has been 449 swept in the set of values: $\{0.01C, 0.1C, C, 10C, 100C\}$. In 450 order to evaluate the influence of v in the number of selected 451 features, we have considered the overall set of values v = i/d, 452 1 < i < d, where d is the data dimension, when v-SP-453 SVM is applied over a predefined feature group, parameter 454 d is replaced by the number of groups G. As for Dr-SVM 455 parameters, λ_1 and λ_2 , they have been selected among the set 456 of values {0.01, 0.1, 1, 10, 100}. 457

In the following discussions, both results evaluating the evolution of the CE and the number of features when ν value is explored, and results achieved when ν value is cross validated, will be analyzed. Additionally, we will include the CE achieved by a new SVM retrained with only the subset of features selected by the ν -SP-SVM methods, in this way, we will check whether the fact of pruning the weights associated to irrelevant features degrades the final model performance. 463

The MOSEK library¹ has been used as optimizer for all 466 algorithms under study.

A. Orange Data Model

As a first simulation problem, we have considered the 469 "orange data" model, which has been previously employed 470 in [29] to test the standard 1-norm SVM performance. In this 471 problem, two standard normal independent random variables 472 x_1, x_2 are generated. Negative class elements of data $[x_1, x_2]^T$ 473 satisfy inequality 4.5 $\leq x_1^2 + x_2^2 \leq 8$, whereas positive 474 elements are distributed along all space \mathbb{R}^2 . Thus, negative 475 class surrounds almost all positive class patterns, like the 476 skin of an orange. Additionally, to check the feature selection 477 ability of the different algorithms, q random independent 478 standard Gaussian inputs have been included in the model. 479 Finally, this input space has been expanded with a second 480 degree polynomial function, i.e., $\{\sqrt{2}x_j, \sqrt{2}x_jx_k, x_j^2, j, k =$ 481 $1, 2, \ldots, 2 + q$ to create a new data set with p new input 482 features. 483

In the experiments, the number of added random features, *q*, has been fixed to 0, 2, 4, 6, 8, 12, and 16 generating an expanded input space of 5, 14, 27, 44, 65, 119, and 189 features. To design the different SVM classifiers, independent and balanced training, validation and test data sets have been generated with 100, 500, and 1000 data, respectively, and each simulation has been repeated 200 times. In this experiment,

²Note that the Bayes boundary is given by $x_1^2 + x_2^2 = 4.5$, therefore, from the overall set of *p* new features, only terms x_1^2 and x_2^2 are useful.

¹MOSEK ApS, Denmark. Available at http://www.mosek.com. The MOSEK Optimization Tools version 6.0 (Revision 61). User's manual and reference, 2010.

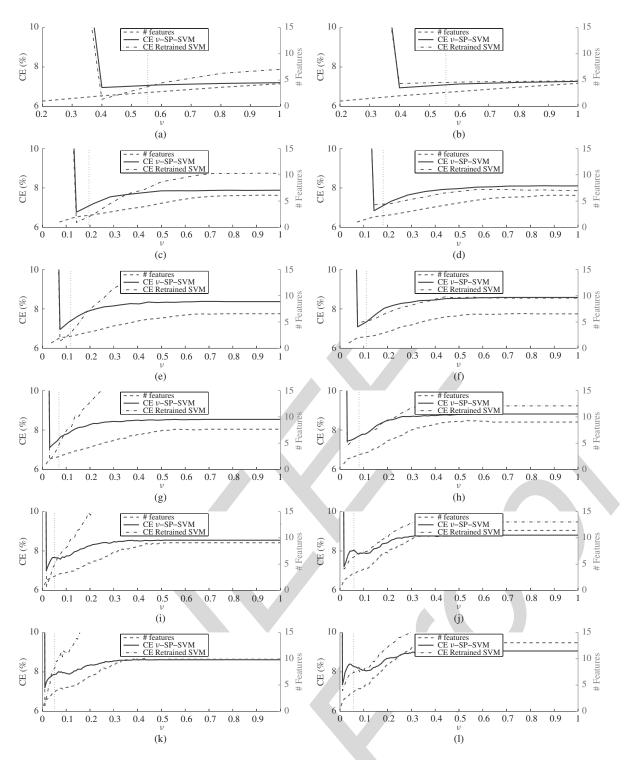


Fig. 1. Evolution of the averaged CE and the averaged number of selected features in ν -SP-SVM methods as a function of ν for orange data set. Dash-dotted line shows the averaged CE of an SVM retrained with the features selected by v-SP-SVM. Dotted vertical line marks the averaged cross-validated v value. (a) 2 norm v-SP-SVM (q = 0). (b) 1 norm v-SP-SVM (q = 0). (c) 2 norm μ -SP-SVM (q = 2). (d) 1 norm v-SP-SVM (q = 2). (e) 2 norm v-SP-SVM (q = 4). (f) 1 norm v-SP-SVM (q = 4). (g) 2 norm v-SP-SVM (q = 8). (h) 1 norm v-SP-SVM (q = 8). (i) 2 norm v-SP-SVM (q = 12). (j) 1 norm ν -SP-SVM (q = 12). (k) 2 norm ν -SP-SVM (q = 16). (l) 1 norm ν -SP-SVM (q = 16).

different SVM free parameters (C, C', and ν) have been 491 optimized using the validation set. 492

The MATLAB code that implements the proposed ν -SP-493 SVM algorithms and a demo, which allows us to replicate 494 the results shown in this section can be downloaded from 495 http://www.tsc.uc3m.es/ hmolina/paper_nu-SP-SVM/. 496

Table I presents the averaged CE rates achieved by the dif-497 ferent SVM methods under study and the number of features in their models. These results show the following.

- 1) Classical SVM methods rise the CE rate and the number 500 of features in the model when q is increased, as it is 501 expected, standard 1-norm SVM and Dr-SVM provide 502
- 498 499

sparser solutions than standard 2-norm SVM, even if 503 some noisy features are included in the final model. 504 Note that Dr-SVM, which penalizes with L1 and L2 505 norms, retains more useless features than 1-norm SVM 506 and, although its performance improves 2-norm SVM, 507 it is not as accurate as 1-norm SVM. 508

The proposed ν -SP-SVM approaches keep the classifi-509 cation error rates around 7%, independently of q and, 510 in most cases, they only employ the useful features: 511 note that the average number of selected features is 512 always very close to 2. However, standard 2-norm SVM 513 uses all original features and standard 1-norm SVM and 514 Dr-SVM tend to include some useless features. 515

3) When 2-norm and 1-norm v-SP-SVM results are com-516 pared to each other, we do not observe relevant differ-517 ences, since they present similar CEs and similar number 518 of features. 519

Fig. 1 depicts the evolution of the averaged classification 520 error and the averaged number of selected features as a 521 function of parameter ν in the orange problem, for each value 522 of ν , parameters C and C' have been adjusted by the validation 523 process. A dotted vertical line indicates the working point 524 of the results from Table I, when ν was also selected in 525 the validation process. Additionally, this figure includes the 526 averaged CE rate, which could be achieved by retraining a 527 new standard SVM with the set of features selected by ν -528 SP-SVMs. This figure shows the following behaviors of the 529 proposed methods. 530

1) As it was expected, ν plays a crucial role to obtain a 531 reduced number of features and an accurate solution. 532 Fixing $\nu = 1$, the provided results would be similar 533 to the standard 1-norm SVM, however, reducing v534 both performance improvements and reductions in the 535 number of model parameters could be achieved, mainly 536 if v was close to 2/d. 537

2) The role of ν as upper bound on the number of selected 538 features is clearly seen. When ν is close to 1, the 539 proposed v-SP-SVM methods do not include all original 540 features in their models, since most noisy features are 541 removed. For instance, when q = 8, 12, or 16, there 542 are 65, 119, and 189 original features, but v-SP-SVMs 543 employ less than 10, 12, or 14 features. 544

Finally, it is important to point out that the model 545 performance is not degraded by pruning the coefficients 546 associated to irrelevant features (those whose slack vari-547 ables γ_i are zero). If we compare the solutions provided 548 by ν -SP-SVM models with a new standard SVM trained 549 with the selected set of features, slight performance 550 improvements could be achieved; but, when any noisy 551 feature is included in the model, the retrained SVM tends 552 to overfit, whereas proposed v-SP-SVM models provide 553 accurate solutions. 554

B. Benchmark Data Sets 555

To test the performance of the proposed ν -SP-SVM clas-556 sifiers over real data sets, 8 benchmark binary classification 557 problems have been selected from the universal communica-558 tions identifier (UCI) repository [38]: Abalone, Credit, Hand, 559

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TABLE II

CHARACTERISTICS OF THE BINARY DATA SETS: NUMBER OF FEATURES AND NUMBER OF DATA BELONGING TO EACH CLASS IN TRAINING AND TEST SETS

Problem	# Features (<i>d</i>)	# Train samples (n_1/n_{-1})	# Test samples (n_1/n_{-1})
Abalone	8	1238/1269	843/827
Credit	15	215/268	92/115
Hand	62	1923/1900	906/891
Image	18	821/1027	169/293
Ionosphere	34	150/84	75/42
Pima	8	188/350	80/150
Spam	57	1218/1847	595/941
Wdbc	30	238/141	119/71

Image, Ionosphere, Pima, Spam, and Wisconsin Diagnostic 560 Breast Cancer (Wdbc). These problems have been chosen 561 because of their diversity in the number of data and dimen-562 sions. The main characteristics of these problems are summa-563 rized in Table II. To adjust the free parameters of the different 564 models, the parameter ranges described in the introduction of the experimental section have been swept by applying a fivefold CV process. 567

For this benchmark analysis we have also included, as 568 an additional reference method, the RFE method from [39]. 569 This algorithm carries out a feature selection process by 570 iteratively removing the feature with less weight in the SVM 571 solution. To fairly compare this method with proposed ν -SP-572 SVM methods, we have implemented the linear version of 573 the RFE algorithm, additionally, the final feature subset of the 574 RFE method is selected with a CV process (note that the RFE 575 method obtains a different feature subset in each iteration) and 576 a new SVM has been trained using only the selected features. 577

Table III shows the results achieved by the different SVM 578 algorithms under study averaged over 50 runs with randomly 579 selected training/validation sets. As it can be observed, stan-580 dard 1-norm SVM fails to remove irrelevant features in some 581 problems. For instance, in Abalone, Pima, and Spam almost 582 all original features are retained. Dr-SVM is worse than the 583 standard 1-norm SVM in this regard, and hardly removes 584 any feature in the considered problems (with the exception 585 of Credit). 586

In contrast, it is possible to perform effective feature 587 selection with the proposed ν -SP-SVMs without incurring in 588 any significant degradation in classification performance. In 589 particular, Table III shows a 25% model complexity reduction 590 in *Image*, Spam, and Wdbc when ν -SP-SVM, as opposed to 591 its standard counterpart, is used. This percentage is even better 592 for other problems, reaching 33.3% in Abalone and Hand and 593 50% in Ionosphere. 594

When we compare the proposed ν -SP-SVM approaches 595 with the RFE method, we observe that the automatic feature 596 selection carried out by our proposals is competitive with stan-597 dard feature selection procedures which have to, first, select 598 the feature subset and, second, train the classifier. According to 599 Table III, results are quite similar for most problems. However, 600

2 AND 1-NORM V-31-5 VIIS IN THE BINAKT CLASSIFICATION I ROBLEMS							
		Standar	d SVM	Dr-SVM	RFE	v-SP	-SVM
			1-norm	D1-3 V W	KI L	2-norm	1-norm
Abalone	CE	21.10(±0.89)	20.51(±0.11)	20.60(±0.14)	20.90(±0.58)	20.90(±0.37)	20.85(±0.34)
Abuione	# feat.	8.00(±0.00)	7.96(±0.20)	8.00(±0.00)	4.34(±2.18)	5.36(±2.11)	5.80(±1.87)
Credit	CE	10.65(±0.10)	11.07(±0.13)	11.07(±0.13)	10.99(±0.21)	10.68(±0.15)	11.02(±0.19)
Creati	# feat.	15.00(±0.00)	1.16(±0.55)	2.08(±3.36)	4.32(±4.83)	7.16(±3.15)	1.36(±0.78)
Hand	CE	9.17(±0.18)	9.24(±0.10)	9.20(±0.12)	9.43(±0.22)	9.15(±0.22)	9.29(±0.21)
Папа	# feat.	62.00(±0.00)	55.68(±4.20)	55.56(±4.08)	34.82(±6.04)	45.72(±4.96)	42.06(±5.67)
Image	CE	14.94(±0.95)	12.94(±0.18)	13.11(±0.23)	14.05(±1.07)	13.18(±0.43)	12.98(±0.19)
Image	# feat.	18.00(±0.00)	13.96(±0.20)	17.24(±0.77)	16.06(±1.49)	14.38(±2.58)	13.52(±1.03)
Ionosphere	CE	11.93(±2.02)	11.73(±2.35)	12.38(±0.85)	13.76(±2.12)	11.79(±1.92)	12.27(±1.08)
Tonosphere	# feat.	33.00(±0.00)	24.42(±7.47)	30.92(±3.29)	13.96(±5.13)	18.32(±6.55)	17.44(±3.90)
Pima	CE	23.63(±0.71)	23.29(±0.22)	23.35(±0.31)	23.78(±1.03)	23.36(±0.33)	23.00(±0.20)
1 tma	# feat.	8.00(±0.00)	7.44(±0.50)	7.76(±0.43)	5.26(±2.04)	6.34(±1.14)	6.72(±1.05)
Spam	CE	6.88(±0.17)	7.15(±0.09)	7.03(±0.06)	6.78(±0.21)	6.99(±0.24)	7.09(±0.15)
Span	# feat.	57.00(±0.00)	54.52(±1.79)	56.22(±0.79)	44.68(±3.03)	44.88(±3.21)	42.88(±3.28)
Wdbc	CE	2.97(±0.92)	4.31(±0.68)	3.19(±0.51)	3.43(±0.57)	3.28(±0.53)	3.77(±0.75)
w ubc	# feat.	30.00(±0.00)	18.52(±3.25)	27.38(±3.17)	21.80(±3.59)	22.64(±2.27)	13.80(±2.70)

TABLE III CE AND NUMBER OF SELECTED FEATURES PROVIDED BY STANDARD 2 AND 1-NORM SVMS, DR-SVM, THE RFE METHOD AND THE 2 AND 1-NORM V-SP-SVMS IN THE BINARY CLASSIFICATION PROBLEMS

in the case of *Image*, both v-SP-SVM proposals outperform the 601 RFE method, and for Credit and Wdbc, the 1-norm v-SP-SVM 602 approach achieves the best accuracy-complexity trade-off. On 603 the other hand, in problems such as Ionosphere or Hand, RFE 604 presents a lower number of features, although this advantage 605 is achieved at the expense of a CE increase. 606

Figs. 2 and 3 show the evolution of the classification 607 error and the number of selected features as a function of 608 ν in the different data sets. A dashed line depicts the CE 609 achieved by new standard SVMs retrained with the set of 610 features selected by the proposed v-SP-SVM models and a 611 dotted vertical line points out the ν value selected in the 612 validation process. These figures remark the clear trade-off 613 between the model complexity and the final CE. In problems 614 such as Credit, Image, Ionosphere, and Wdbc, when the 615 1-norm ν -SP-SVM is applied, we could directly have fixed 616 $\nu = 1$, and most useless features would have been removed. 617 However, an adequate selection of v is crucial to obtain an 618 accurate solution. The validation process has carried out a 619 conservative selection of parameter ν , if, during the validation 620 process, a slight performance degradation had been allowed, a 621 additional features would have been removed, in fact, for all 622 the problems under study but *Credit*, lower values of v would 623 have resulted in a lower number of features, while keeping 624 similar error rates. Finally, it is important to note that the 625 retraining procedure does not show any clear improvement, 626 since although in some cases the final CE is slightly improved, 627 in other cases it is similar or, even, slightly worse. 628

C. High Dimensional Datasets 629

The aim of this section is to test the performance of the 630 proposed methods when we are dealing with a large number 631 of input features. For this purpose, the Dexter dataset [40] 632

has been considered. The goal of this problem is to classify 633 texts about "corporate acquisitions" into two categories. The 634 data set has 20000 features, from which 9947 variables 635 correspond to a "bag-of-words" representation of several texts 636 and the remaining 10 053 features are noisy features added 637 to complicate the classification task. The different data set 638 partitions are balanced with 300 training data, 300 validation 639 patterns and 2000 test samples. 640

Due to the large number of input features, the CV of all possible ν values in the ν -SP-SVM methods is not reasonable. For this reason, we have followed this strategy.

- 1) We have first trained the proposed methods with $\nu = 1$, 644 what provides a first approximation to the number of useful features. In this case, 1-norm ν -SP-SVM achieves 646 a CE = 8.1% with only 150 features and 2-norm v-SP-SVM a CE = 6% with 3976 variables.
- 2) According to above number of selected features, the 649 maximum value of ν , worthy of being explored, has been 650 fixed. For instance, in 1-norm ν -SP-SVM this value has 651 been fixed to 0.01 (150 is less than the 1% of 20 000) 652 and in 2-norm ν -SP-SVM has been set to 0.2 (3976 is 653 close to the 20% of 20 000). 654
- 3) Then, a range of 10 linearly spaced ν values has been defined. In particular, ranges $\{0.1\%, 0.2\%, \ldots, 1\%\}$ and $\{2\%, 4\%, \ldots, 20\%\}$ have been explored by each v-SP-SVM model.
- 4) Finally, the optimum ν value has been selected as the one with minimum validation error.

As a result of this procedure, 1-norm ν -SP-SVM has selected 661 a v value of 0.004, achieving a CE = 7.75% with only 662 79 features, whereas 2-norm ν -SP-SVM has used a final ν 663 value of 0.1 providing a CE of 6.4% with 1487 features. 664 Reference methods, 2-norm, 1-norm, and Dr-SVMs, have 665

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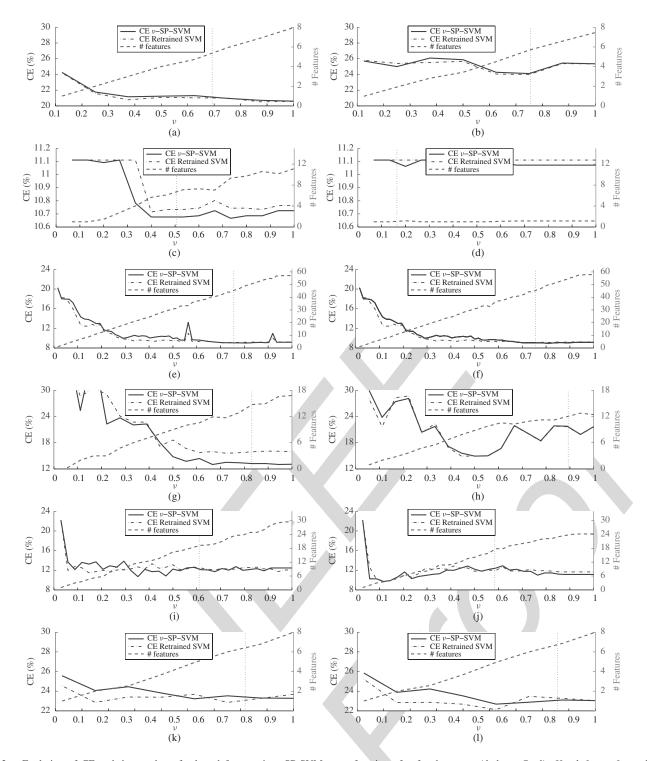


Fig. 2. Evolution of CE and the number of selected features in v-SP-SVMs as a function of v for data sets: *Abalone, Credit, Hand, Image Ionosphere*, and *Pima*. Dash-dotted line shows the CE of an SVM which has been retrained with the features selected by v-SP-SVM model. Dotted vertical line marks the cross-validated v value. (a) 2-norm v-SP-SVM *Abalone*. (b) 1-norm v-SP-SVM *Abalone*. (c) 2-norm v-SP-SVM *Credit*. (d) 1-norm v-SP-SVM *Credit*. (e) 2-norm v-SP-SVM *Hand*. (g) 2-norm v-SP-SVM *Image*. (h) 1-norm v-SP-SVM *Image*. (i) 2-norm v-SP-SVM *Ionosphere*. (j) 1-norm v-SP-SVM *Ionosphere*. (k) 2-norm v-SP-SVM *Pima*. (l) 1-norm v-SP-SVM *Pima*.

presented *CEs* of 6.45%, 8.10% and 6.05%, respectively, and they have used 7142, 159, and 5750 features (see Table IV). These results show that 1-norm ν -SP-SVM outperforms standard 1-norm SVM by achieving a lower *CE* with half the number of features. Regarding 2-norm ν -SP-SVM and standard 2-norm SVM, they present similar error rates, but the latter is using 35% of the features instead of 7.43% used by 2-norm ν -SP-SVM. Finally, Dr-SVM provides the lowest *CE*, but the number of selected features (5750) is much higher than the 1487 of the 2-norm ν -SP-SVM.

Besides, it is important to point out that 1-norm-based algorithms (standard 1-norm SVM and 1-norm ν -SP-SVM) 677

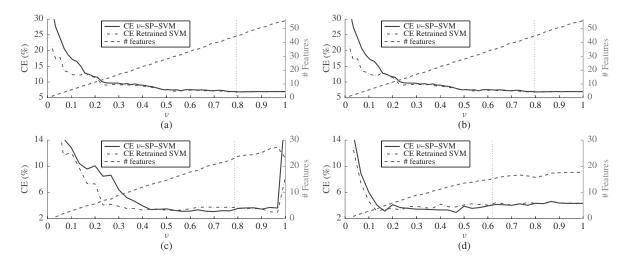


Fig. 3. Evolution of CE and the number of selected features in v-SP-SVMs as a function of v for data sets: *Spam* and *Wdbc*. Dash-dotted line shows the CE of an SVM which has been retrained with the features selected by v-SP-SVM model. Dotted vertical line marks the cross-validated v value. (a) 2-norm v-SP-SVM *Spam*. (b) 1-norm v-SP-SVM *Spam*. (c) 2-norm v-SP-SVM *Wdbc*. (d) 1-norm v-SP-SVM *Wdbc*.

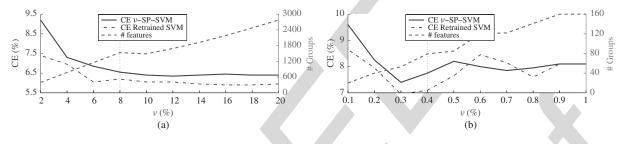


Fig. 4. CE and the number of selected features in ν -SP-SVM algorithms as a function of ν in *Dexter* data set. Dash-dotted line shows the CE of an SVM which has been retrained with the features selected by ν -SP-SVM model. Dotted vertical line marks the cross-validated ν value. (a) 2-norm ν -SP-SVM. (b) 1-norm ν -SP-SVM.

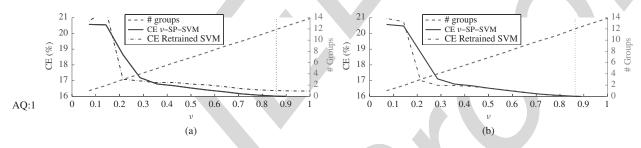


Fig. 5. Evolution of CE and the number of selected features in v-SP-SVMs as a function of v for data sets: *Spam* and *Wdbc*. Dash-dotted line shows the CE of an SVM which has been retrained with the features selected by v-SP-SVM model. Dotted vertical line marks the cross-validated v value. (a) 2-norm v-SP-SVM *Spam*. (b) 1-norm v-SP-SVM *Spam*. (c) 2-norm v-SP-SVM *Wdbc*. (d) 1-norm v-SP-SVM *Wdbc*.

have selected a few number of features, prompting a performance degradation. This effect is due to the fact that the
maximum number of features that can be selected is always
upper bounded by the number of training data [30], [32]. For
this reason, these approaches are working with few hundreds
of features instead of selecting thousands as the 2-norm-based
methods.

Finally, Fig. 4 shows the evolution of the *CE* and the number of features in the model for the explored range of ν values. At first glance, it can be seen that, in the explored range of ν , values larger than 8% in 2-norm ν SP-SVM and 0.3% for 1-norm ν SP-SVM are able to provide accurate results with a low number of features, even lower than 1-norm, 2-norm, and Dr-SVM methods. This figure also shows the *CE* achieved

TABLE IV CE and Number of Selected Features Provided by Different Methods Under Study in Dexter Data Sets

			Standard SVM		v-SP-SVM	
		2-norm	1-norm	Dr-SVM	2-norm	1-norm
Derter	CE	6.45	8.10	6.05	6.4	7.75
Dexter	# feat.	7142	159	5750	1487	79

when the SVM is retrained with the selected set of features, 692 suggesting that, in problems where the number of removed features is high, the retraining process is able to provide an additional advantage in terms of *CE* reduction. 692

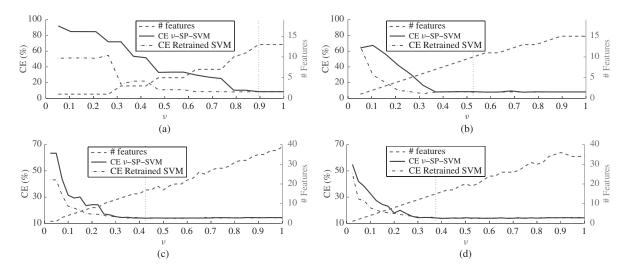


Fig. 6. Evolution of the CE and the number of selected features in ν -SP-SVM algorithms as a function of ν in multiclass problems. Dash-dotted line shows the CE of an SVM which has been retrained with the features selected by ν -SP-SVM model and dotted vertical line marks the cross-validated ν value. (a) 2-norm ν -SP-SVM *Segmentation*. (b) 1-norm ν -SP-SVM *Segmentation*. (c) 2-norm ν -SP-SVM *Wave*. (d) 1-norm ν -SP-SVM *Wave*.

TABLE V PREDEFINED FEATURE GROUPS IN THE PROBLEM ADULT. CATEGORICAL FEATURES ARE CODIFIED WITH DUMMY VARIABLES

# group	Original feature	Categorical / continous	# of categories	# of features in each group
1	age	continuous	_	1
2	workclass	categorical	8	3
3	fnlwgt	continuous	-	1
4	education	categorical	16	4
5	education-num	continuous	-	1
6	marital-status	categorical	7	3
7	occupation	categorical	14	4
8	relationship	categorical	6	3
9	race	categorical	5	3
10	sex	categorical	2	1
11	capital-gain	continuous	-	1
12	capital-loss	continuous	-	1
13	hours-per-week	continuous	-	1
14	native-country	categorical	41	6

696 D. Selecting Feature Groups with v-SP-SVM

To analyze the performance of the proposed methods when 697 features need to be selected according to predefined sets, 698 instead of selecting isolated features, we have chosen the 699 dataset Adult from [38]. The aim of this problem is to 700 determine whether a person earns over 50K a year from 701 several demographic characteristics from 14 original features, 702 of which six are continuous and eight are categorical. Each 703 categorical feature has been coded with dummy variables, 704 using N indicatrix variables (0 or 1) to codify their 2^N 705 possible values, in this way, each data is finally represented 706 by 33 features belonging to 14 groups as it is described in 707 Table V. Then, when a group selection approach is applied, the 708 dummy variables representing to the same categorical feature 709 will be either all selected or all removed from the final model. 710 Note that only when all variables from a certain group are 711

removed it is possible to skip the capture of the associated categorical variable.

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This binary data set has 30162 training samples and 15060 714 data to test the model. To train the different SVMs, we have 715 randomly selected a 10% of the original training data set, 716 therefore, 3016 data have been used to train the different meth-717 ods. A 5-fold CV process has been applied to adjust the free 718 parameters of the different methods and their performances 719 have been evaluated over whole test data. The different SVMs 720 have been trained 100 times, with different randomly selected 721 training data, and their averaged results have been studied. 722

As result, standard 2 and 1-norm SVMs present an averaged 723 CE of $16.33(\pm 0.3)\%$ and $15.97(\pm 0.2)\%$ employing 14 and 724 13.9 ± 0.3 groups, respectively, whereas Dr-SVM presents 725 the same performance (both in CE and number of selected 726 features) as 1-norm SVMs. This result is a consequence of 727 standard 2-norm SVM having selected all groups and 1-norm 728 SVM and Dr-SVM having seldom discarded group 10, this 729 group is associated to original feature sex and codified with 730 only one dummy variable. 731

To compare these results with the proposed methods, Fig. 5 732 depicts the values of the CE and the number of selected 733 groups as a function of parameter ν in ν -SP-SVMs. It can 734 be seen that if ν is cross validated (see dotted vertical line), 735 ν -SP-SVMs present CE close to 16% with 12 groups, since 736 groups 3 and 10 are usually removed. However, if we had 737 wanted to select a lower number of groups, v could have 738 been fixed around 0.3, keeping the CE lower than 17% and 739 selecting just the 4 most relevant groups: Groups associated to 740 original features education-num, relationship, and capital-gain 741 are always chosen and additionally, either group 4 (education) 742 or 7 (occupation) is included in the model. Thus, this example 743 illustrates the convenience of the ν formulation of SP-SVM for 744 allowing a more flexible selection of the number of variables 745 to be incorporated in the model. 746

Again, a retraining process (dash-dotted line in Fig. 5) $_{747}$ provides a small improvement, since for most ν values, $_{748}$ ν -SP-SVMs, and retrained SVMs achieve similar CEs. $_{749}$

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		Classical SVMs		Dr-SVM	Sparse SVMs	
		2-norm	1-norm	DI-5 V IVI	2-norm	1-norm
Segmentation	CE	9.05	9.00	8.24	8.43	8.52
	# feat.	18.00	13.00	15	13.00	10.00
Wave	CE	13.87	14.33	14.20	13.87	14.07
	# feat.	40.00	38.00	30.00	17.00	15.00

TABLE VI CE and Number of Selected Features Provided by Different Methods Under Study in Multiclass Data Sets

750 E. Multiclass Problems

In this section, we will test the performance of the 751 v-SP-SVMs over multiclass datasets Segmentation and Wave 752 from the UCI repository [38]. The purpose of Segmentation 753 problem is to classify hand-segmented images represented by 754 19 features in 7 categories: brickface, sky, foliage, cement, 755 window, path, and grass. The data set has 210 and 2100 756 training and test data, respectively. Wave problem consists of 757 3 classes of waves to be identified from 40 features, whose 758 latter 19 ones are all noise, the data set has 3500 training 759 samples and 1500 test data. As in the previous sections, the 760 free parameters of the different methods have been adjusted 761 with a 5 fold CV process. 762

To train the different classifiers, proposed ν -SP-SVM meth-763 ods have solved problem (10), either in its 2-norm or in its 764 1-norm version, whereas reference methods have directly used 765 the multiclass problem defined by (9) with their corresponding 766 penalization terms. Table VI presents the results achieved by 767 both standard and proposed SVMs. As it can be observed, 768 ν -SP-SVMs achieve lower error rates with lower number of 769 features. In Segmentation, CE is reduced in a 0.5%, with 770 respect to 1-norm and 2-norm SVMs, using only 13 and 771 10 features, whereas Dr-SVM achieves a slightly lower CE 772 using 15 features. In Wave, the advantages of the proposed 773 SVM classifiers are clearer, since the number of features in 774 the model is half the number for the reference methods and 775 the CE is similar in the 2-norm models, slightly reduced in 776 the 1-norm methods and Dr-SVMs are outperformed by both 777 v-SP-SVMs. 778

⁷⁷⁹ When the evolution of CE and the number of features are ⁷⁸⁰ analyzed as a function of ν (see Fig. 6), the trade-off between ⁷⁸¹ these parameters is again observed. Besides, retrained SVMs ⁷⁸² provide a significant CE reduction in *Segmentation* problem.

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V. CONCLUSION

This paper introduced a method for feature selection based 784 on a new formulation of linear SVMs that includes constraints 785 additional to the classical ones. These constraints drop the 786 weights associated to those features that are likely to be 787 irrelevant. In order to predefine an upper bound for the number 788 of relevant features, a v-SVM formulation has been used, 789 where ν is a parameter that indicates the fraction of features 790 to be considered. This parameter is swept in an efficient 791 way in order to find the optimal number of features over 792 a validation set of data. This paper presented two versions 793

of the formulation, the first one being an SVM with a 2-794 norm regularization term. The second one uses a 1-norm 795 regularization, that has a reduced computational burden with 796 respect to the first one. Besides, this new SVM formulation 797 allows us to easily apply the feature selection process over 798 predefined feature sets. This, in turn, is useful to introduce a 799 straightforward, yet efficient way to extend the algorithms to 800 multiclass problems. 801

Experiments showed that the introduced methods present advantages not only in terms of CE, but also in the ability of reducing the model complexity by adequately removing features during the training process, not as a preprocessing stage. Also, these experiments showed that the algorithms are efficient when applied to the task of feature group selection and to multiclass problems.

Future research includes nonlinear versions of the algorithm in order to take into account the nonlinear relationships between features. Applications can also include extensions to regression problems as well as linear model selection for signal processing tasks, such as filter design or plant modeling, in situations where optimal models are known to be sparse.

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