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Selection of Tuning Parameter in L1-Support Vector Machine via. Particle Swarm Optimization Method

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Abstract: Descriptor selection for classification methods is one of the most important topics in the chemometrics. The selection of descriptors can be considered to be a variable selection problem that aims to find a small subset of descriptors that has the most discriminative information for the classification target. Penalized Support Vector Machine (PSVM) is one of the most effective embedded methods and it is more preferable than the Support Vector Machine (SVM) because PSVM combines the standard SVM with a penalty to simultaneously perform both variable selection and classification. The PSVM with L1-norm is the most widely used methods. However, the efficiency of PSVM with L1-norm depends on appropriately choosing the tuning parameter which is involved in the L1-norm penalty. In this study, a particle swarm optimization method which is a metaheuristic continuous algorithm is proposed to determine the tuning parameter in PSVM with L1-norm penalty. The proposed method will efficiently help to find the most significant descriptors in constructing Quantitative Structure–Activity Relationship classification (QSAR) model with high classification performance. Depend on the four datasets, the experimental results show the favorable performance of the proposed method when the number of descriptors is high and the sample size is low comparing with other competitor methods.

Key words: QSAR, L1-norm, classification, penalized support vector machine, particle swarm optimization, cluster

INTRODUCTION

With the development of technologies in the chemometrics, large volumes of chemical data are generated, presenting a challenge for chemometricians to conduct the statistical classification. One of these challenges is the low number of observations (chemical compounds) and the large number of variables (descriptors) (Al Fakih *et al*., 2016). High dimensionality of the data affects the performance of any used classifier due to the presence of irrelevant, noisy and redundant variables. These uninformative variables may dominate the informative variables for classification.

Variable selection which is also known as dimensionality reduction is the method of selecting an optimum subset of relevant variables that can improve the performance of statistical classification and to avoid the curse of dimensionality (Khajeh *et al*., 2012). Consequently, several variable selection methods have been proposed and studied in the literature. These methods can be divided into three broad categories: The filter, wrapper and embedded methods (Algamal and Lee, 2015).

Filter methods are one of the most popular variable selection methods which are based on a specific criterion by gaining information of the each variable. These methods are work separately and they are not dependent on the classification method. For the wrapper methods, on the other hand, the variable selection process is based on the performance of a classification algorithm to optimize the classification performance. In embedded methods, variable selection process is incorporated into the classification methods which can simultaneously perform variable selection and classification (Liang *et al*., 2013). Support Vector Machine (SVM) has attracted much substantial attention from many statisticians in recent years because of its theoretical and practical advantages that justify its improved performance in classification (Shen *et al*., 2007). The main objective of the SVM is to find a hyper-plane which effectively separates between two classes of data points to identify a decision boundary with the maximum geometric margin (Cong *et al*., 2013). Despite the excellent characteristics of SVM, there are still several drawbacks including the selection of variables. In other words, SVM cannot perform variable selection (Zhu *et al*., 2004). Penalized Support Vector Machine (PSVM) which is one of the most effective embedded methods is more preferable than the SVM because PSVM combines the standard SVM with a penalty to simultaneously perform both variable selection and classification (Wang *et al*., 2008). With deferent penalties, numerous PSVMs can be applied, among them is L1-norm which is known as the least absolute shrinkage and selection operator (lasso) (Broman and Speed, 2002).

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However, the efficiency of PSVM with L1-norm depends on appropriately choosing the tuning parameter which is involved in the L1-norm penalty. The tuning parameter controls the tradeoff between classification and the number of selected variables. As a result, selecting a suitable value of the tuning parameter is an important part of fitting. The most widely used approach for selecting the tuning parameter is Cross-validation (CV) which is a data-driven approach. However, it was pointed out that CV usually identify too many irrelevant variables when the number of variables is large and can be very time consuming (Park *et al*., 2014).

In this study, a particle swarm optimization method which is a metaheuristic continuous algorithm is proposed to determine the tuning parameter in PSVM with L1-norm penalty. The proposed method will efficiently help to find the most significant variables in constructing quantitative structure-activity relationship classification model with high classification performance. The experimental results show the favorable performance of the proposed method when the number of variables is high and the sample size is low.

MATERIALS AND METHODS

Support vector machine: Support vector machine is an excellent, efficient, effective and a powerful classification method for binary classification problems which is based on the statistical learning theory (Dong and Jian, 2015).

Support vector machine has several important advantages: great flexibility, high accuracy, ability of generalization, computational efficiency, high performance when the number of variables is large and dealing with complex nonlinear problems using a simple linear algorithm by using soft margin approach (Bi *et al*., 2003). Training SVM is equivalent to solving the problem of convex linear constrained quadratic programming. SVM is based on mapping the sample observations into a high-dimensional feature space to search and obtain an optimal separating hyperplane which maximizes the sum of the distances between two classes in this space (Liu *et al*., 2010).

In chemometrics application, descriptor matrix can be described as a matrix X = $(x_{ij})_{n\times d}$ where each column represents a descriptor and each row represents a sample (compound). The numerical value of x_{ij} denotes the value of a specific descriptor J (j = 1,…, d) in a specific sample i(= 1,…, n). For a binary classification problem, given a training dataset $\{(x_i,y_i)\}_{i=1}^{n}$ where, $x_i = (x_{i,j}, x_{i,2},\ldots, x_{i,d})$ represents a vector of the ith descriptor and $t_i \in \{-1, +1\}$ for i = 1,…, n where, y_i = +1 indicates the ith sample is in class 1 and y_i = -1 indicates the ith sample is in class 2.

An SVM generates a real-valued function φ(X) as a hyperplane to maximize the distance, w, between the data which should be separated. There exists two parallel boundaries φ(X).w+b = ∓1 which can exactly separate two classes. The separating hyperplane, sgn(φ(x).w+b), is between them. The margin between these two boundaries is defined as 2/||w||. In order to maximize this margin, the following problem must be solved as:

$$\begin{aligned}&\min_{w,b}\frac{1}{2}w^{T}w\\&\text{S.T.}\quad y_i(\varphi(x_i)\ w_i+b)\geq 1,\quad i=1,2,\ldots,n.\end{aligned}\qquad(1)$$

By solving this problem, the optimal hyperplane $\text{sgn}((\tilde{w}\times x)+\tilde{b})$ of Eq. 1 with a solution of $\tilde{w}$ and $\tilde{b}$ are obtained.

Depending on Lagrangian, Eq. (1) can be written as a quadratic dual optimization problem by:

$$\begin{aligned}&\min_{\alpha}\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j x_i^{T}x_j-\sum_{i=1}^{n}\alpha_i\\&\text{S.T.}\quad \sum_{i=1}^{n}\alpha_i y_i=0,\quad \alpha_i\geq 0\ ,\quad i=\ 1,\ 2,\ldots,n\end{aligned}\qquad(2)$$

Where:

α : A vector of Lagrange multipliers vector
α_i : Corresponds to a training observation (x_i, y_i)

Equation 1 and 2 are used for linearly separable training observations. However, to extend the SVM for the linearly non-separable training observations, each observation (x_i, y_i) is associated with a slack variable $\zeta_i \geq 0$. The constraint in Eq. 1 becomes $y_i(\varphi(x_i)w_i+b)+\zeta_i \geq 0$. Thus Eq. 1 becomes:

$$\begin{aligned}&\min_{w,\,b}\frac{1}{2}w^{T}w+C\sum_{i=1}^{n}\zeta_i\\&\text{S.T.}\quad y_i(\varphi(x_i)\ w_i+b)+\zeta_i\geq 1,\quad i=1,2,\ldots,n\end{aligned}\qquad(3)$$

where C is a parameter that controls the tradeoff between the maximum margin and the minimum classification error. Then, the Lagrangian becomes:

$$\begin{aligned}&\min_{\alpha}\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j K(x_i.x_j)-\sum_{i=1}^{n}\alpha_i\\&\text{S.T.}\quad \sum_{i=1}^{n}\alpha_i y_i=0,\quad 0\leq\alpha_i\leq C\ ,\quad i=\ 1,\ 2,\ldots,n\end{aligned}\qquad(4)$$

where, $K(x_i.x_j) = \varphi(x_i)^{T}\ \varphi(x_j)$ is the kernel function that allows the maximum margin to be applied efficiently in high-dimensional feature space.

Penalized support vector machine: Although SVM has been proven useful in binary classification, it cannot perform features selection because of using L2-norm, $\| w \|_2^2$. Typically, any classification problem includes a number of features where many of these features can be noisy or redundant, leading to degrade the performance of the classification algorithm. Therefore, reducing dimensions is an essential step that can be achieved through feature selection strategies.

Bradley and Mangasarian (1998) and Zhu *et al.* (2004) proved that the SVM optimization problem is equivalent to a penalization problem which has the form:

$$\min_{w,b} \frac{1}{n}\sum_{i=1}^{n}\left[1-y_i f(x_i)\right]_+ + \mathrm{Pen}_\lambda(w) \qquad (5)$$

where, $[1\text{-}y_i \ f(x_i)]_+ = \max(1\text{-}y_i \ f(x_i), 0)$ represents the hinge loss term and Pen_λ (w) represents the penalty term. Several penalties have been proposed. Among them, L_1-norm (Zhu *et al.*. 2014; Bradley and Mangasarian, 1998), L_q-norm with q<1 (Liu *et al*., 2010; Ikeda and Murata, 2005; Liu *et al*., 2007). Furthermore, Zhang, *et al.* (2005) proposed the Smoothly Clipped Absolute Deviation (SCAD) penalty of Fan and Li (2001) with SVM. In addition, Wang, *et al*. (2008) proposed a hybrid huberized SVM by using the elastic net penalty while Becker, *et al.* (2011) proposed a combination of ridge and SCAD with SVM.

The L1-norm penalty, proposed by Bradley and Mangasarian (1998) and Zhu *et al*. (2004) is one of the most popular penalty function because SVM with L_1-norm can automatically select features by shrinking the hyper-plane coefficients to zero. The SVM-L1 is defined as:

$$\min_{w,b} \frac{1}{n}\sum_{i=1}^{n}\left[1-y_i f(x_i)\right]_+ + \lambda\sum_{j=1}^{d}| w_j | \qquad (6)$$

where, λ is a positive tuning parameter which controls the amount of shrinkage. Equation 6 is a convex optimization problem and can be solved by the method of Lagrange multipliers.

Particle swarm optimization method: Particle Swarm Optimization (PSO) is a nature-inspired metaheuristic algorithm that was originally proposed by Kennedy and Eberhart (1995) for solving continuous optimization problems.

The PSO inspires the social or collective behavior of animals such as bird flocking and fish schooling. PSO compares with the other computation intelligence-based algorithms has several advantages such as simple implementation, computationally higher efficiency, fewer parameters to tune, scalability and flexibility, robustness. For instance, comparing with genetic algorithm, there is no crossover and mutation genetic operation (Chen *et al*., 2014; Kiran, 2017; Lin *et al*., 2008; Lu *et al*., 2011; Zhou and Dickerson, 2014).

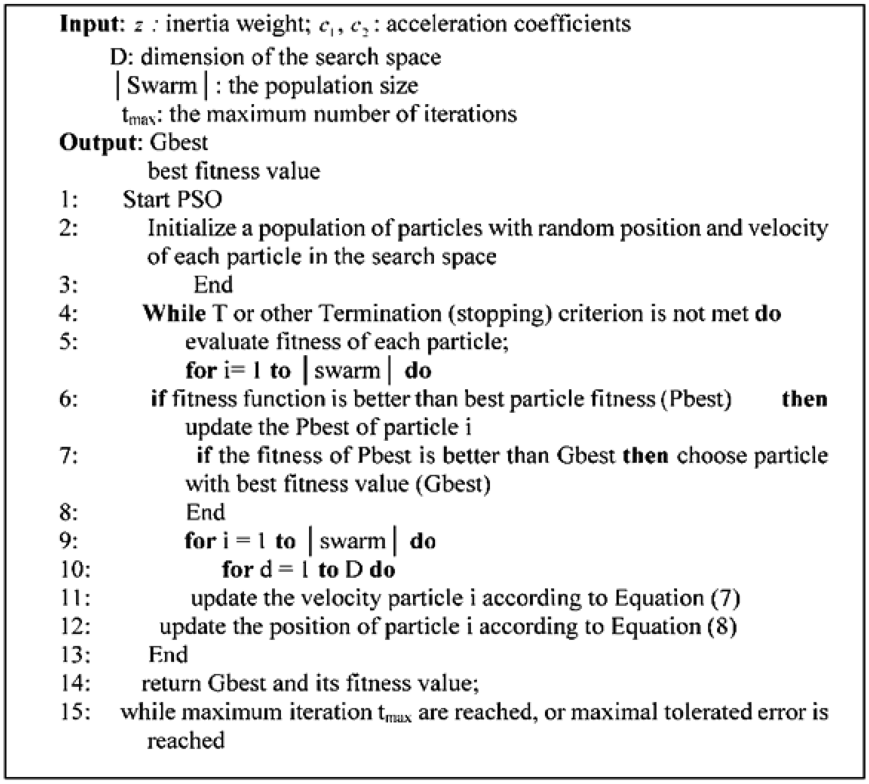
The PSO performs the searching using a population which is called swarm, of particles. Each particle has three features: position, velocity and fitness value. In PSO, each particle can be represented as a candidate solution (position) in the search space. The particles fly through the search space by their own efforts and in cooperation with other particles and they follow the best solutions they have achieved (local best solutions) as well as tracking the best solutions that they found (the best global solution) (Cervantes *et al*., 2017; Lai *et al*., 2016; Mirjalili and Lewis, 2013; Wen *et al*., 2011).

Mathematically, the search space is assumed to be D-dimensional and there are m of particles in the swarm where d = 1, 2…, D. During the movement, each particle has a position vector $x_i = \{x_{i1}, x_{i2},\dots, x_{id}\}$ with a velocity vector $v_i = \{v_{i1}, v_{i2},\dots, v_{id}\}$. In the PSO algorithm, the best position which gives the best fitness value for the particle i is called best previous position denoted as $\mathrm{Pbest}_i = \{\mathrm{Pbest}_{i1}, \mathrm{Pbest}_{i2},\dots, \mathrm{Pbest}_{id}\}$. The best position found by all particles is called the global best which is denoted as $\mathrm{Gbest}_i = \{\mathrm{Gbest}_{i1}, \mathrm{Gbest}_{i2},\dots, \mathrm{Gbest}_{id}\}$. In each iteration, the PSO algorithm searches for the optimal solution by updating the position and the velocity of the ith particle according to the following two equations:

$$v_{id}^{t+1} = z \times v_{id}^{t} + c_1 \times r_1 \times \left(\mathrm{Pbest}_{id}^{t} - x_{id}^{t}\right) + c_2 \times r_2 \times \left(\mathrm{Gbest}_{id}^{t} - x_{id}^{t}\right) \qquad (7)$$

where, t denotes the iteration in the algorithm, z is the inertia weight which is used to balance between the global search and the local search. In addition, c_1 (the cognition learning factor) and c_2 (social learning factor) are the acceleration coefficients. While r_1 and r_2 are random values selected from a uniform distribution with (0,1). The pseudo code of the PSO algorithm is displayed in Fig. 1.

Proposed method: The efficiency of penalized support vector machine with L1-norm penalty largely depends on an appropriately choosing the tuning parameter, λ. In the penalization, λ controls the tradeoff between classification and the number of selected features. As a result, it is of crucial importance selecting a suitable value of the λ. A choice of λ that is small leads to overfitting the data because a large number of variables will not be removed. While when λ is large, a large number of variables will be removed.



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Input: $z$ : inertia weight; $c_1$, $c_2$ : acceleration coefficients
      D: dimension of the search space
      |Swarm| : the population size
      $t_{max}$: the maximum number of iterations
Output: Gbest
        best fitness value
  Start PSO
    Initialize a population of particles with random position and velocity
    of each particle in the search space
      End
    While T or other Termination (stopping) criterion is not met do
      evaluate fitness of each particle;
      for i= 1 to |swarm| do
    if fitness function is better than best particle fitness (Pbest)    then
      update the Pbest of particle i
        if the fitness of Pbest is better than Gbest then choose particle
      with best fitness value (Gbest)
      End
      for i = 1 to |swarm| do
        for d = 1 to D do
        update the velocity particle i according to Equation (7)
      update the position of particle i according to Equation (8)
    End
    return Gbest and its fitness value;
  while maximum iteration $t_{max}$ are reached, or maximal tolerated error is
    reached
```

Fig. 1: Pseudo code of the PSO algorithm

In literature, the most widely used method for selecting λ is the Cross-Validation (CV), which is a data-driven approach. However, it was pointed out that CV usually identify too many irrelevant variables when the number of variables is large (Broman *et al*., 2002; Chen *et al*., 2014) and can be very time consuming (Park *et al*., 2014). Consequently, several modification of the CV approach in estimating λ have been suggested by researchers (Roberts and Nowak, 2014; Sabourin *et al*., 2015; Jung and Hu, 2015; Meijer and Goeman, 2013; Pang *et al*., 2016).

Due to drawbacks of CV approach, in this study, a PSO algorithm is proposed to determine the tuning parameter in PSVM with L1-norm penalty. The proposed method will efficiently help to find the most significant variables in constructing quantitative structure-activity relationship classification model with high classification performance. The parameter configurations for our proposed method are presented as follows.

The number of particles, m is set to 50 and the number of iterations is t_{max} = 100. The acceleration coefficients c_1 and c_2 are set within the range (Khajeh *et al*., 2012; Liang *et al*., 2013). The c_1 and c_2 are updating during the iteration according to the following equations:

$$c_1 = c_{1,min} + \frac{t}{t_{max}}(c_{1,max} - c_{1,min}) \quad (9)$$

$$c_2 = c_{2,min} + \frac{t}{t_{max}}(c_{2,max} - c_{2,min})$$

Further, the minimum and the maximum values for the inertial weight are: z_{min} = 0.2 and z_{max} = 0.9. The inertial weight is updating according to the following equation:

$$z = z_{max} - \frac{t}{t_{max}}(z_{max} - z_{min})$$

The positions of each particle are randomly determined. The position of a particle represents the tuning parameter, λ. The initial positions of the particles are generated from a uniform distribution within the range (0-100). The initial velocities of each particle are generated from a uniform distribution within the range (0, 4). The fitness function is defined as:

$$\text{Fitness} = 0.8 \times \text{CA} + 0.2 \times \left(\frac{d-q}{d}\right)$$

Table 1: Characteristics of the four used datasets

Datasets	Compounds No. (n)	Descriptors No. (p)	Class
Dataset 1	212	2571	Active = 108/inactive = 104
Dataset 2	75	3067	inhibitor = 108/non-inhibitor = 104
Dataset 3	121	2559	31 active/90 inactive
Dataset 4	479	2322	213 active/266 weakly active

where, CA is the classification accuracy that obtained, d represents the number of descriptors in the dataset, q represents the number of the selected descriptors. The fitness function are calculated for all particles and the Pbest and Gbest vectors are determined.

The velocities and positions are updated using Eq. 7 and 8, respectively. Steps 4 and 5 are repeated until a tmax is reached.

Evaluation criteria: The classification performance of the used methods was measured by Classification Accuracy (CA), Sensitivity (SE), Specificity (SP), Mathew's Correlation Coefficient (MCC) and Area under the Curve (AUC). The used criteria are defined as:

$$\text{CA (\%)} = \frac{\text{TP+TN}}{\text{TP+FP+FN+TN}}\times 100\% \qquad (13)$$

$$\text{SE (\%)} = \frac{\text{TP}}{\text{TP+FN}}\times 100\% \qquad (14)$$

$$\text{SP (\%)} = \frac{\text{TN}}{\text{FP+TN}}\times 100\% \qquad (15)$$

$$\text{MCC} = \frac{\text{(TP+TN)-(FP+FN)}}{\sqrt{\text{(TP+FP)(TP+FN)(TN+FP)(TN+FN)}}} \qquad (16)$$

where TP, TN, FP and FN be the numbers of true positive, true negative, false positive and false negative of the confusion matrix, respectively. The higher value of the used evaluation criteria the power classification performance is.

Datasets: Four collected datasets that are binary classification problem and that have different numbers of descriptors and compounds are collected. Dragon Software (Version 6.0) was used to generate 4885 molecular descriptors including all 29 blocks based on the optimized molecular structures. Preprocessing steps were carried out to include consistent and useful descriptors. The first step is to discard the descriptors that had zero values. Then, remove the descriptors that had constant value for all compounds. After that, the descriptors in which 90% of their values were zeros were removed. Finally, descriptors with a relative standard deviation of <0.001 were deleted.

The four datasets are: diverse series of antimicrobial agents dataset which contains 212 different agents with 2571 descriptors. The corresponding antimicrobial activities were measured as pMIC (the logarithm of reciprocal of minimum inhibitory) concentration against CA. The median (ME) of all 212 pMICs (ME = 1.3) as a cutoff value to classify these antimicrobial agents into active (>1.3, n=108) or inactive (<1.3, n = 104) is considered as in Daszykowski *et al*. (2004) and Xing *et al.* (2014). This dataset consists of 75 compounds with HDAC8 inhibitory activity and 3067 descriptors. According to the IC_{50} (half maximal inhibitory concentration) values, the compounds are divided into two classes: An inhibitor class (0.008 μM $<IC_{50}\leq 0.3$ μM) containing 38 compounds and a non-inhibitor class ($IC_{50}>0.3$ μM) containing 37 compounds (Cao *et al*., 2015). A dataset of 121 molecules of thiourea derivatives with anti-HCV activity and 2559 descriptors was used by Algamal *et al*. (2017). According to their experimental EC_{50} (the concentration of a drug that gives half-maximal response), the molecules were divided into two categories by the threshold value of 0.1 μM: actives ($EC_{50}<0.1$ μM) and inactives ($EC_{50}\geq 0.1$ μM). This dataset measures 2322 descriptors corresponding to 479 neuraminidase inhibitors of in uenza a viruses (H1N1). The compounds were separated into two groups according to their IC_{50}: active compounds with $IC_{50}<20$ μM and those with $IC_{50}\geq 20$ μM were considered as weakly active compounds (Algamal and Lee, 2015; Li *et al*., 2016). The main characteristics of four datasets are summarized in Table 1.

RESULTS AND DISCUSSION

With the aim of correctly assessing the performance of our proposed method, PSVM-PSO, comparative experiments with the original CV of estimating the tuning parameter (PSVM-CV) and the modified CV of Jung and Hu (2015) (PSVM-MCV) were carried out.

In these experiments, a 10-fold is set and the range of the tuning parameters for the used methods is fixed with 0 and 100. In addition, the linear kernel function is employed. To obtain a reliable classification performance, for each dataset, a 70% of samples is used as a training dataset and remaining 20% of the samples is used as a testing dataset. This partition repeated 20 times and the averaged evaluation criteria are reported in Table 2.

As can be seen from Table 2, PSVM-PSO selected less descriptors than the PSVM-MCV and PSVM-CV for all the datasets. In dataset 4 (neuraminidase inhibitors of

Table 2: Classification performance (on average) of the methods used over 20 partitions. The number in parentheses is the standard error

		Training dataset					Testing dataset
Datasets	Methods	Selected descriptors (No.)	CA	SE	SP	MCC	CA
Dataset 1	PSVM-PSO	48 (0.087)	97.04 (0.038)	96.52 (0.032)	95.80 (0.035)	0.964 (0.037)	94.83 (0.041)
	PSVM-MCV	57 (1.02)	92.22 (0.371)	90.92 (0.374)	91.31 (0.372)	0.915 (0.371)	89.07 (0.411)
	PSVM-CV	73 (1.11)	90.35 (0.381)	90.51 (0.387)	90.31 (0.375)	0.901 (0.382)	87.57 (0.408)
Dataset 2	PSVM-PSO	31 (0.117)	96.22 (0.121)	94.74 (0.124)	93.68 (0.123)	0.958 (0.121)	93.21 (0.217)
	PSVM-MCV	49 (0.741)	92.72 (0.214)	91.12 (0.236)	91.36 (0.242)	0.918 (0.252)	89.85 (0.266)
	PSVM-CV	55 (1.113)	91.90 (0.355)	89.93 (0.372)	92.66 (0.441)	0.908 (0.361)	87.36 (0.402)
Dataset 3	PSVM-PSO	40 (0.002)	98.68 (0.005)	96.54 (0.006)	95.84 (0.006)	0.977 (0.003)	96.22 (0.008)
	PSVM-MCV	51 (0.081)	92.24 (0.061)	91.87 (0.061)	92.32 (0.065)	0.911 (0.065)	88.34 (0.074)
	PSVM-CV	59 (0.092)	90.74 (0.071)	90.11 (0.077)	90.34 (0.073)	0.898 (0.078)	87.11 (0.085)
Dataset 4	PSVM-PSO	59 (0.071)	98.82 (0.066)	97.24 (0.071)	97.32 (0.069)	0.979 (0.071)	95.81 (0.088)
	PSVM-MCV	105 (0.255)	91.35 (0.236)	89.20 (0.238)	92.64 (0.243)	0.905 (0.244)	87.37 (0.274)
	PSVM-CV	416 (1.013)	88.64 (0.516)	87.84 (0.538)	86.71 (0.537)	0.881 (0.522)	84.21 (0.614)

Table 3: Friedman and Bonferroni test results for the used methods over the four datasets

Methods	Friedman average rank	Friedman test results	Bonferroni test results
PSVM-PSO	4.058	$\chi^2_{\text{Friedman}} = 16.036$, p-value (0.05) = 0.0011	$\alpha_{0.05} = 6.185$
PSVM-MCV	8.186		$\alpha_{0.01} = 6.185$
PSVM-CV	11.385		$\alpha_{0.10} = 6.185$

influenza a viruses (H1N1)), for instance, PSVM-PSO selected 59 descriptors compared to 105 and 416 descriptors for PSVM-MCV and PSVM-CV, respectively. Importantly, PSVM-PSO had the potential to select less descriptors than the other two methods, indicating that most of these additionally selected descriptors were probably not highly irrelevant to classification study.

In terms of classification accuracy, PSVM-PSO achieved a maximum accuracy of 97.04, 96.22, 98.68 and 98.82% for dataset 1, 2, 3 and 4, respectively. Furthermore, it is clear from the results that PSVM-PSO outperformed the PSVM-CV in terms of classification accuracy for all datasets. This improvement in classification accuracy is mainly due to the PSVM-PSO ability in selecting the tuning parameter. Moreover, PSVM-MCV slightly improved the classification accuracy compared to PSVM-CV. The improvements were 2.027, 0.887, 1.161 and 2.966% for the dataset 1, 2, 3 and 4, respectively.

It can easily observe from Table 2 that PSVM-PSO has the best results in terms of the sensitivity and specificity. The PSVM-PSO has the largest sensitivity of 95.80, 93.68, 95.84 and 97.32% for the dataset 1, 2, 3 and 4, respectively. This indicated that PSVM-PSO significantly succeeded in identifying the compounds that in fact are active (or inhibitor) with a probability of 0.958, 0.936, 0.958 and 0.973, respectively. On the other hand, the results for the specificity represent the probability of a PSVM-PSO in identifying the compounds that are inactive (or non-inhibitor). In terms of the SP, PSVM-PSO significantly outperformed the PSVM-MCV and PSVM-CV for all datasets. In the dataset 4, for example, PSVM-PSO has the largest probability of 0.973 in identifying the inactive compounds compared to 0.926 and 0.867 for PSVM-MCV and PSVM-CV, respectively.

Looking at the Mathew's correlation coefficient, the classification performance of the PSVM-PSO is comparable with PSVM-MCV and PSVM-CV performing best among them. In dataset 3, the MCC value was 0.977 of PSVM-PSO which is higher than that of PSVM-MCV (MCC = 0.911) and PSVM-CV (MCC = 0.898). In general, an algorithm with a higher Mathew's correlation coefficient value is considered to be a more predictive classification algorithm.

Further, depending on the testing dataset, the PSVM-PSO achieved the best classification results for the four datasets. In the same line, the PSVM-MCV appears in the second position. In contrast with the results, PSVM-CV attains poor classification results. For instance, in dataset 2, the CA of the testing dataset is 93.21% by the PSVM-PSO which is higher than 89.85 and 87.36% by PSVM-MCV and PSVM-CV, respectively.

Depending on the AUC criteria, a non-parametric Friedman test was employed to check whether the PSVM-PSO, PSVM-MCV and the PSVM-CV were statistically significant. Then, the post hoc of Bonferroni test was computed when the null hypothesis is rejected. This test is computed under different critical values (0.01, 0.05 and 0.1). Table 3 summarized the statistical test results. Based on the obtained results, the null hypothesis is rejected at 0.05 significance level using Friedman test statistic. As a result, the obtained results showed statistically significant differences between the PSVM-PSO and the other two used methods. In addition, the PSVM-PSO has the lowest average rank with 4.058 comparing with PSVM-MCV and the PSVM-CV. Depending on Bonferroni test results, it is clearly obvious that the average ranks of PSVM-MCV and PSVM-CV are higher than $\alpha_{0.05}$, $\alpha_{0.01}$ and $\alpha_{0.10}$. These results suggesting that both PSVM-MCV and PSVM-CV are significantly worse than PSVM-PSO over the four datasets.

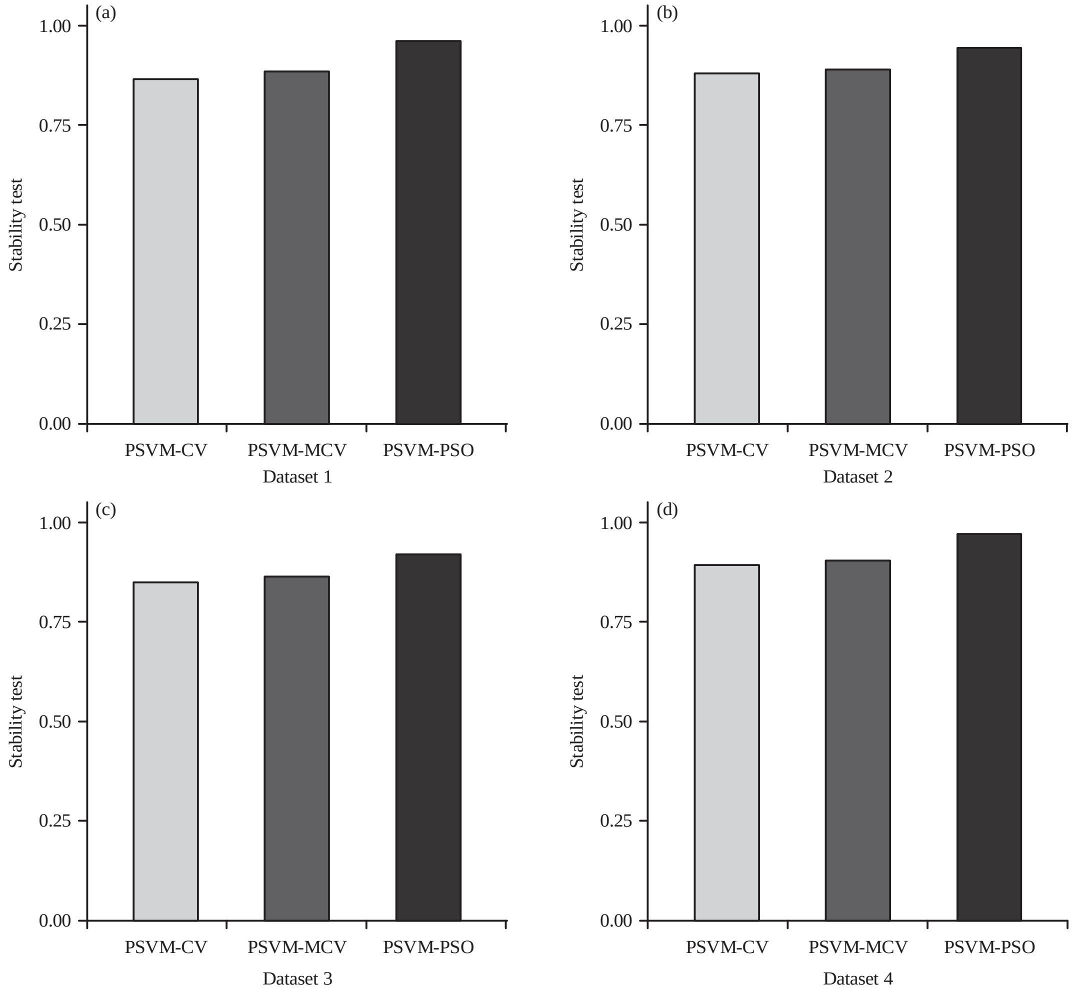

Fig. 2(a-d): Stability test results of the used methods for the four datasets

Further, a stability test which is an indicator of descriptor selection consistency, using the Jaccard index is utilized to highlight the performance of the PSVM-PSO.

Let, D_1 and D_2 be subsets of the selected descriptors such that $D_1, D_2 \subseteq D$, for a number of solutions $D = \{D_1, \ldots, D_r\}$, the stability test is defined as:

$$\text{Stability test} = \frac{2}{r(r-1)} \sum_{i=1}^{r-1} \sum_{j=i+1}^{r} I_J(D_i, D_j) \qquad (17)$$

where, $I_j(D_i, D_j)$ is the Jaccard index which is defined as the size of the intersection between any two groups divided by the size of their union. Mathematically, it is defined as:

$$I_J(D_1, D_2) = \frac{|D_1 \cap D_2|}{|D_1 \cup D_2|}$$

The higher the stability test value is, the more stable the descriptor selection is. Figure 2 shows the stability test values on the four datasets for the PSVM-PSO, PSVM-MCV and the PSVM-CV. As can be seen from Fig. 2, the PSVM-PSO displays the high rate of stability compared with PSVM-MCV and PSVM-CV.

CONCLUSION

This study has proposed a PSO algorithm for determining the tuning parameter of penalized support vector machine with L1-norm. Results obtained from t he PSVM-PSO are compared with PSVM-MCV and PSVM-CV. Experimental results with the four dataset suggest that the PSVM-PSO choose the tuning parameter consistently which reduces the dimensionality of the datasets efficiently and improves the classification performance.

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