Invited Paper

Prediction of Abnormal Wine Fermentations Using Computational Intelligent Techniques*

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ABSTRACT

The early detection abnormal fermentations (sluggish and stuck) is one of the main problems that appear in wine production, due to the significant impacts in wine quality and utility. This situation is specially important in Chile, which is one of the top ten worldwide wine production countries. In last years, two different methods coming from Computational Intelligence have been applied to solve this problem: Artificial Neural Networks and Support Vector Machines. In this work we present the main results that have been obtained to detect abnormal wine fermentations applying these approaches. The Support Vector Machine method with radial basis kernel present the best results for the time cutoffs considered (72 [hr] and 96 [hr]) over all the techniques studied with respect to prediction rates and number of the training sets.

Keywords: Abnormal, Wine Fermentations, Artificial Neural Networks, Support Vector Machines.

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1. INTRODUCTION

In 2011, the wine production of 10.46 million hectoliters have placed Chile as one of the top ten wine-producing countries and among the top five major wine-exporting countries, see refs. [1, 2]. The quality of the chilean wine is one of the key factor that explain that explain these results. The wine quality can be affected in all stages of the winemaking process but particularly at the fermentation step. In the case of Chile, approximately 1% to 5% of wine fermentation processes fail because of problems causing stuck and sluggish fermentations. Stuck or incomplete alcoholic fermentations are defined as those leaving a higher than desired residual sugar content in the wine once the yeast has ceased to act. Winemakers consider a complete or "dry" fermentation as one containing less than 0.2% to 0.4% residual sugar, which is equivalent to 2 to 4 g/L of C5 and C6 sugars, see ref. [3]. On the other hand, a sluggish fermentation occurs when the yeast is struggling to ferment (late-onset), see ref. [4], and it can potentially stop fermenting altogether and become stuck, see ref. [5]. Slow fermentation is recognized by a low fermentation rate throughout the process, see ref. [4].

Considering only losses in raw materials (grapes), the cost is approximately USD 43,200 per fermentation (USD 0.7–2.0/kg of grapes on average, and 32 tons/fermentor). Additionally, some fermentations have problems during their development, but they are corrected and the fermentations finish normally. However, the quality of these fermentations could be affected because of the increased time of fermentation and/or because of the corrective actions that were taken. At the moment, fermentations are identified as problematic only when the rate of sugar uptake is either too slow or has stopped altogether, see ref. [3]. Unfortunately, in some cases, at that time, it is too late to easily rescue the fermentation. Hence, the ability to improve the prediction horizon for problematic fermentations would enable winemakers to take timely corrective actions and significantly reduce winery losses, see ref. [4]. The current literature relating to problematic wine fermentations is substantial. Factors such as high initial sugar content, extreme temperature or pH, lack of nutrients such as nitrogen or oxygen, high ethanol content, competition from other microorganisms, short- and medium-chain fatty acids, and incorrect enological practices (see refs. [3,4,6-9]) have all been considered as the main causes of fermentation problems.

2. ARTIFICIAL NEURAL NETWORKS APPLIED TO PREDICT ABNORMAL WINE FERMENTATIONS

The field of Computational Intelligence refers to heuristics methods that come from Artificial Intelligence, such as Artificial Neural Networks, Support Vector Machines, Fuzzy Logic and Evolutionary Computation, among others, see refs. [10-13]. These heuristics are designed using an approach based on learning, adaptation, evolution techniques in order to solve complex computational problems, like the ones that appear in Combinatorial Optimization and Pattern Recognition. The methods most used on this field are Artificial Neural Networks (ANN), Support Vector Machines (SVM) and Genetic Algorithms. In general, the first two ones are applied in tasks that appear in Pattern Recognition, such as: Classification, Identification, Clustering, Regression, etc., see refs. [11-13]. Different authors have proposed using hybrid computational intelligence heuristics for pattern recognition problems, see refs. [14,15], as well as for implementing hybrid heuristics constructed with methods coming from computational intelligence and statistical learning [16]. Two hybrid methods based on ANN and evolutionary computation for the construction and optimization of network topology and interaction weights are called evolutionary neural networks [15]. Both methods show competitive performance in real-world classification and regression problems in comparison with other data-mining algorithms.

An Artificial Neural Network (ANN) is a model of a biological neural network that exhibits the main capabilities of the real system: parallel processing, classification, learning and pattern recognition. These capabilities allow them to detect complex relationships between inputs and outputs, recognize patterns and reproduce the behavior of a system after a previous training stage with known data, see refs [11,12]. An ANN is completely characterized by: a vector of input and output states, a connectivity matrix, a bias or threshold vector, a transition function, a network architecture and a learning rule. After a previous training and testing stage with known data, the ANN have shown in numerous applications the ability to detect complex relationships between inputs and outputs, to recognize patterns and to model the behavior of a system, see refs [11,12]. This ability strongly depends on the correct choice of: the architecture of the ANN, the learning algorithm, the activation functions and the characteristics of the data set. The ANN method has been widely used for modeling nonlinear dynamical systems in many applications such as classification and identification, fault detection as well as process control and optimization.

In wine production, the applications of ANN have been concentrated in the identification and classification processes, see ref. [17-21]. Penza and Cassano (ref. [19]) chemometrically classified different classes of Italian wines using a multisensor array and different ANN algorithms. The best results obtained with respect to the recognition rate and prediction rate were 100% and 78%, respectively. Both statistical and ANN methods were used to classify 70 Spanish rose wines that had different denominations of origin, see ref. [20]. From 19 variables studied, the statistical method (SLDA) chose 10 variables and obtained a global percentage of correct classification of 98.8% and a percentage of correct prediction of 97.3%, while the ANN method chose 7 variables and obtained a correct classification for training and prediction of 100%. In ref. [21] a multilayer perceptron technique was applied in order to classify 36 Slovak wine samples of 3 varieties, produced by 4 producers in 3 different years with respect to the variables: variety, producer/location and the year of production. At least it was obtained a 93.3% prediction performance over the samples considered.

In refs. [22, 23] was studied the application of ANNs to early detected abnormal wine fermentations. In the experiments were used a database that contains approximately 22000 data of industrial fermentations of Cabernet Sauvignon which come from 22 normal, sluggish and stuck fermentations of Cabernet Sauvignon. The main characteristics of this study were the following:

- Applying mid-infrared spectroscopy and standard methods, were measured for each fermentation 30 to 35 samples of each of the relevant chemical variables for this kind of process: sugars (glucose, fructose), alcohols (glycerol, alcoholic degree), organic acids (tartaric, citric, lactic, malic, acetic, succinic), nitrogen compounds (ammonium and aminoacids) and density.
- Different sub-cases were studied by varying the predictor chemical variables and the time of fermentation: 72, 96 and 256 hrs.
- A multilayer perceptron architecture was selected for the ANN model, which was composed of one input layer with neurons corresponding to predictor variables and one or two hidden layers. The sigmoid function was the communication medium, and one output layer with two neurons represented the dependent variables (1: normal fermentations; 0: abnormal fermentations). The training algorithm was back-propagation with gradient descent.Two parameters were varied, namely the number of layers and the number of neurons that compose each of the layer
- The cases studied consider the training and test phases with 70 and 30% of the fermentations, respectively, and each set of samples (training and test) contained 50% of normal and problematic (stuck and sluggish) fermentations.

In this work was demostrated by several computational experiments that ANNs can be applied to detected at 72 hrs. abnormal wine fermentations with a prediction rate of 100% using only three chemical variables: sugar, ethanol, and density. In Figure 1 is shown an schema of the multilayer feed-forward ANN that was use in ref. [22].

3. SUPPORT VECTOR MACHINES APPLIED TO PREDICT ABNORMAL WINE FERMENTATIONS

Support Vector Machines (SVM) are also one of the most used methods that are currently applied in Pattern Recognition tasks, specially in classification and regression, see refs. [13, 24, 25]. A SVM is a decision method that computes the border that divides the diferent classes in which

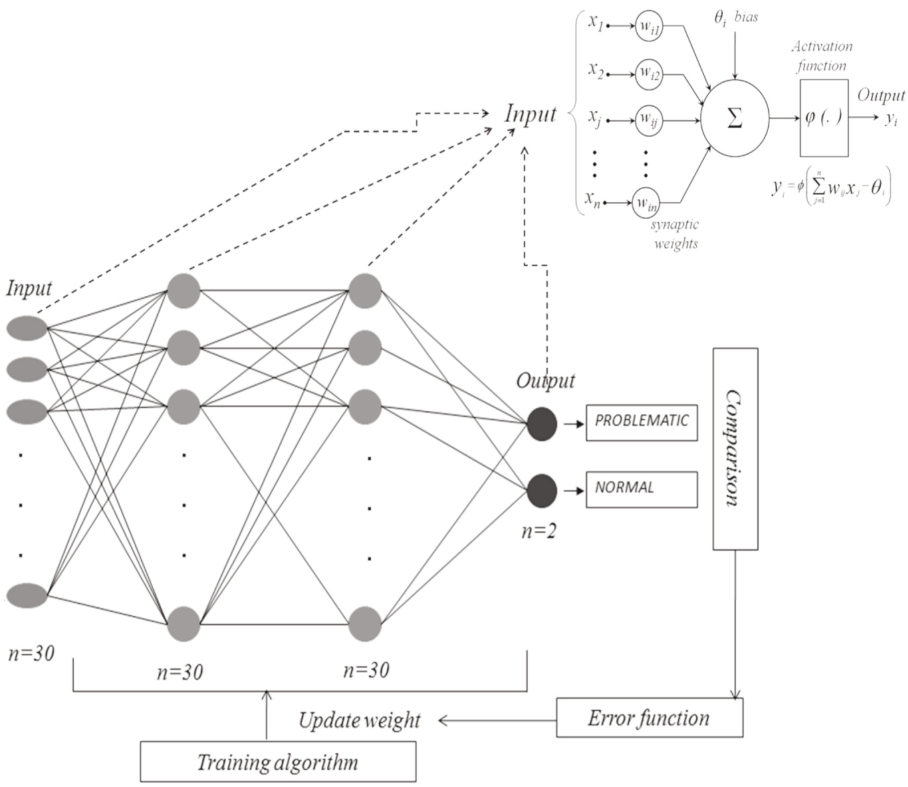

Figure 1: Schema of a multilayer feed-forward ANN with 2 hidden layers, such the one applied in ref. [22].

a set of data is organized. In the case of two clases, the training data, i.e. the vectors and clases, consists of $(n+1)$ dimensional points: $(x_1, y_1), ..., (x_m, y_m)$ where: $x_i \in \mathbb{R}^n$ and $y_i \in \{-1, 1\}$. The SVM method solves the following optimization problem:

$$\begin{array}{l} \min\limits_{w,b,\varepsilon} \left(\frac{1}{2} w^t w + c \sum\limits_{i=1}^{m} \varepsilon_i^p \right) \\ \text{s.t.} \\ y_i \left(w^t \phi(x_i) + b \right) \geq 1 + \varepsilon_i \quad \forall i = 1, ..., m \\ \varepsilon_i \geq 0 \quad \forall i = 1, ..., m \end{array} \tag{1}$$

Where the function $\phi(u)$ defines the kernel $K(u, v)$ of the method, in the following sense:

$$K(u, v) = \phi^t(u)\phi(v) \tag{2}$$

The most commonly used functions $K(u, v)$ are the linear, polynomial with degree d and radial basis function kernels, which are defined respectively by :

$$\begin{array}{l} K(u, v) = u^t v \\ K(u, v) = (u^t v + 1)^d \\ K(u, v) = \exp\left(-\gamma \left\| u - v \right\|^2 \right) \end{array} \tag{3}$$

The objective function in (1) minimizes the distance between borders that divide the different classes and the classification error. The constant $c > 0$ can be interpreted as a penalization parameter: a small value of c allows to increase the separation between borders, while a big value of c allows to reduce the classification error. The values of the parameters b, c are determined experimentally using the training set, see refs. [13, 24, 25]. The SVM method has been applied to several biotechnology problems with great success, such as: determination of the rice wine composition by means of Vis–NIR spectroscopy, see ref. [26], DO classification of spanish white wines, see ref. [27], bird species recognition, see ref. [28], detection of meat and bone meal in compound feeds, see ref. [29].

In ref. [30], it was applied the SVM method to detect abnormal wine fermentations with three different kernels: linear, third degree polynomial and radial basis function. For the training and testing phase, it was used the same database of ref. [22].

- The percentage of training and testing data was set to 80% - 20%, 70% - 30% and 60% - 40%. For the training phase was chosen a fraction of normal, sluggish and stuck fermentation, with the aim of give to the SVM the necessary information for learning.

- A Pyhton program was developed for computing the prediction rate of the SVM methods considered. The library *sklearn*, with the module *svm* has been used; this package enable us to define a training set for the SVM to use, with a corresponding kernel (linear, polinomial or radial basis function) and predict the class for a given input. The program computes the best prediction rates using the data of the main chemical variables (total sugar, alcoholic degree, density) and considering all of the training combinations, given the training and testing percentage (60% - 40%, 70% - 30%, 80% - 20%), the time cutoff (72 hrs., 96 hrs.) and the SVM kernel (linear, polynomial, radial basis).

- The computations were designed in function of the percentage for training and testing set in the following sense: for each fermentation class, the total number is divided according to the percentage; for instance, in the case of 60% - 40%, the normal class (8 fermentations in total) is split in 5 fermentations for training and 3 fermentations for testing, the sluggish class (10 fermentations in total) is split in 6 fermentations for training and 4 fermentations for testing and the stuck class (4 fermentations in total) is split in 2 fermentations for training and 2 fermentations for testing. Then, it is computed all the possible training combinations considering these partitions. For 60% - 40% the number of training combinations $TC(60, 40)$ are is:

$$TC(60, 40) = \binom{8}{3}\binom{10}{4}\binom{4}{2} = 70560 \quad (4)$$

  In the same way, the training combinations are computed for 70% - 30% and 80% - 20%, obtaining $TC(70, 30) = 13440$ and $TC(80, 20) = 1440$.

The main result obtained in ref. [30] establishes that the SVM method, with radial basis function as kernel predicts correctly 100% of fermentation behavior at 72 and 96 hours for all the training and testing percentages. In addition, the results of ref. [22] were improved because all possible training/testing configuration were evaluated. In Table 1 are shown the best prediction rates obtained for the radial basis and polynomial kernels considering the most relevant chemical variables: Total Sugar, Alcoholic Degree, Density.

Training/	Time	SVM Method	
Testing %	Cutoff	Polynomial	Radial Basis
80/20	72 [hr]	75%	100%
	96 [hr]	83%	100%
70/30	72 [hr]	75%	100%
	96 [hr]	83%	100%
60/40	72 [hr]	75%	100%
	96 [hr]	83%	100%

Table 1. Prediction rates for the radial basis an polynomial kernels applied with different training and testing percentages and time cutoffs, see ref. [30].

4. CONCLUSIONS

In this work, we present the main results that have been obtained to predict abnormal wine fermentations by applying Artificial Neural Networks (ANN) and Support Vector Machines (SVM). For the computational experiments we have used a database with approximately 22000 points of 22 normal, sluggish and stuck fermentations. A multilayer perceptron architecture with two hidden layers was implemented for the ANN model and for the SVM was considered three different kernels: linear, third degree polynomial and radial basis function. For both approaches it was computed the best prediction rates using the data of the main chemical variables (total sugar, alcoholic degree, density), considering different training combinations, and time cutoffs.

Our main result establishes that the SVM method with radial basis function kernel is the best method with respect to predictions rates, computing performance and amount of data needed. The result clearly demonstrates that it is possible to obtain valuable information about the fermentation process at 72 hours with a training and testing percentage 80% - 20%. An important future work arises, first: obtain more data in order to study the robustness of the SVM method with radial basis kernel, and second: build an hybrid adaptative method that detect correctly, as early as possible, abnormal wine fermentations.

5. REFERENCES

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