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APLICATIONS OF NEURAL NETWORKS TO FIND THE IMPACT OF WATER IN DIFFERENT BERRY COMPONENTS IN GRAPES

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Abstract: *Grape juice composition during the different stages of berry growth was compared. The analytical data collected were used to investigate the relationships between some of the different components studied in these berries during the ripening period.*

Our goal is to study, with neural networks, the impact of water availability on Vitis vinifera L. cv. Tempranillo grape yields and juice composition over a three-year period.

Keywords: Clustering, Grapes, Neural networks, Organic acids, Sugars, Vitis vinifera.

ACM Classification Keywords: C.1. Processor Architectures , I.5.2 Design Methodology

Introduction

The object of the present study is to ascertain whether irrigation, which has a quantitative effect on the values of the different components analysed in berries of the Tempranillo (Vitis vinífera L.) grape variety, though that effect is not always significant [Esteban MA, Villanueva MJ and Lissarrague JR, 1999], [Esteban MA, Villanueva MJ and Lissarrague JR, 2001] affects the relationships between the different components considered.

We use neural networks models with analysis of sensibility. This model predict more accurately the relationship existing.

The purpose of irrigation is to offset crop water deficits and thereby maximize yields and must quality, to increase profits [Rühl EH and Alleweldt G, 1985]. There are many regions with dry summers in Spain in which irrigation is an effective mean of regulating water availability to grape vines.

As has previously been noted by other workers [Williams LE and Matthews MA, Grapevine, 1990], irrigation of grape vines affects vine physiology, which may directly or indirectly affect yield and grape composition (°Brix, pH, total acidity, etc.) two aspects that also influence wine quality. There is considerable controversy in the literature concerning the positive and negative effects of vine irrigation on must and wine quality [Van Zyl JL, 1984].

Response to irrigation will depend upon such factors as harvest time, crop load, soil water availability and primarily summer rainfall.

Sugar concentration is used as an indicator of fruit maturity, being glucose and fructose the principal sugars in grape juices [Ough CS and Amerine MA, 1988]. Irrigation has a variable effect on sugar accumulation in the berries, and an increase, a decrease, or no change in sugar concentration have all been observed [Hardy P.J.,1968]. The sugar to acidity ratio parameter is ordinarily useful in evaluating the ripening period [Ribéreau-Gayon J, Peynaud E, Ribéreau-Gayon P and Sudraud P, 1975]. Both titratable acidity and pH are of great importance for grape juice stability and are parameters commonly used as an indicator of quality. This is because the concentration of organic acids does not only contributes to the acid taste of the must but also influences subsequent wine color and microbiological stability [Boulton RB, 1980]. According to Hrazdina et al. [Hrazdina G, Parsons GF and Mattick LR, 1984] changes in the pH of grape berries are caused by the metabolism of the major acids and the accumulation of cations, which transform free acids into their corresponding salts. Some authors [McCarthy MG, Cirami RM and McCloud P, 1983], [Romero EG, Muñoz GS and Ibañez MDC, 1993] have stated that decreases in titratable acidity are primarily due to losses in malic acid concentration and to the formation of potassium salts. Potassium is the main mineral cation in grapes [Peynaud E and Ribéreau-Gayon J, 1971], and is predominantly involved in neutralization of tartaric acid and malic acid in the berries, thereby affecting the acid characteristics of the grapes [Hale CR, 1977].

Neural networks can predict any continuous relationship between inputs and the target. Similar to linear or non-linear regression, artificial neural networks develop a gain term that allows prediction of target variables for a given set of input variables. Physical–chemical relationships between input variables and target variables may or may not built into the association of target and input variables.

Neural networks [Anderson, James A. and Edward Rosenfield., 1988] are non-linear systems whose structure is based on principles observed in biological neuronal systems [Hanson, Stephen J. and David J. Burr. 1990]. A neural network could be seen as a system that can be able to answer a query or give an output as answer to a specific input. The in/out combination, i.e. the transfer function of the network is not programmed, but obtained through a training process on empiric datasets. In practice the network learns the function that links input together with output by processing correct input/output couples. Actually, for each given input, within the learning process, the network gives a certain output that is not exactly the desired output, so the training algorithm modifies some parameters of the network in the desired direction. Hence, every time an example is input, the algorithm adjusts its network parameters to the optimal values for the given solution: in this way the algorithm tries to reach the best solution for all the examples. These parameters we are speaking about are essentially the weights or linking factors between each neuron that forms our network.

Neural Networks application fields are typically those where classic algorithms fail because of their inflexibility (they need precise input datasets). Usually problems with imprecise input datasets are those whose number of possible input datasets is so big that they cannot be classified. A field where classic algorithms are in troubles is the analysis of those phenomena whose mathematical rules are unknown. There are indeed rather complex algorithms which can analyses these phenomena but, from comparisons on the results, it comes out that neural networks result far more efficient: these algorithms use Fourier's transform to decompose phenomena in frequential components and for this reason they result highly complex and they can only extract a limited number of harmonics generating a big number of approximations. A neural network trained with complex phenomena's data is able to estimate also frequential components, this means that it realizes in its inside a Fourier's transform even if it was not trained for that.

With neural networks is possible to predict, analyzing historical series of datasets just as with these systems but there is no need to restrict the problem or use Fourier's transform. A defect common to all those methods it is to restrict the problem setting certain hypothesis that can turn out to be wrong. We just have to train the neural network with historical series of data given by the phenomenon we are studying [Anderson, James A. and Edward Rosenfield., 1988.].

Calibrating a neural network means to determinate the parameters of the connections (synapses) through the training process. Once calibrated there is needed to test the network efficiency with known datasets, which has not been used in the learning process. There is a great number of Neural Networks [Anderson, James A. 1995] which are substantially distinguished by: type of use, learning model (supervised/non-supervised), earning algorithm, architecture, etc. Multilayer perceptrons (MLPs) are layered feed forward networks typically trained with static backpropagation. These networks have found their way into countless applications requiring static pattern classification. Their main advantage is that they are easy to use, and that they can approximate any input-output map. In principle, backpropagation provides a way to train networks with any number of hidden units arranged in any number of layers. In fact, the network does not have to be organized in layers any pattern of connectivity that permits a partial ordering of the nodes from input to output is allowed. In other words, there must be a way to order the units such that all connections go from earlier (closer to the input) to later ones (closer to the output). This is equivalent to stating that their connection pattern must not contain any cycles. Networks that respect this constraint are called feed forward networks; their connection pattern forms a directed acyclic graph or dag.

Materials And Methods

Plant material

This experiment was conducted during three consecutive years in a vineyard planted with Richter 110 rootstock and grafted to Vitis vinifera L., cv. Tempranillo. The vineyard was located at the experimental fields of the Polytechnic University of Madrid. Vine spacing was 2m between rows and 1.35m within the row (3700 vines per hectare). Row orientation was North-South. All vines were head trained and cane-pruned (Guyot), and shoots were positioned with a vertical shoot positioning trellis system.

Irrigation treatments

Two irrigation regimes were established: irrigated (I) and non-irrigated (NI) vines. The object was to replace weekly vineyard evapotranspiration (ETc) in the soil from the earliest stages of plant growth, which has depended of when the precipitation took place, as it has been described previously [Esteban MA, Villanueva MJ and Lissarrague JR, 1999]. The potential evapotranspiration (ET0) was calculated from a class A pan evaporation [Doorenbos J and Pruitt WO, 1977]. Daily trickle irrigation was applied at 0.6 x ET0 in the irrigated treatment (I), and no water was applied in the non-irrigated treatment (NI) over the entire growing season. Precipitation amounts less than 5 mm were ignored, and the irrigation application efficiency was considered to be 90%. The soil at this site had a water availability of 131 mm/m. Data on seasonal and annual rainfall, effective rainfall, total water applied, irrigation period, and accumulated growing degree days (10ºC basis) from budbreak to harvest have been described in an earlier paper [Esteban MA, Villanueva MJ and Lissarrague JR, 1999].

Four replications of each of the two treatments were randomly distributed in the vineyard, each replication consisting of three rows with nine vine plots. Measurements were made on the central seven vines of the middle row.

Analytical determinations

General variables: Total soluble solids (ºBrix) was measured using an Abbé type refractometer (Zeiss, mod.B) equipped with a temperature control system (20ºC). Must pH was measured with a pH meter (Crison mod. MicropH 2001), using a glass electrode. Finally, titratable acidity was measured by titration with a base to an end point of pH=8.2 (20ºC), and the results were expressed in g/L tartaric acid.

Glucose and fructose: Analysis of these two sugars was performed by HPLC according to the procedure described by Esteban et al. [Esteban MA, Villanueva MJ and Lissarrague JR, 1999].

The chromatograph employed was equipped with a refractive index detector (Waters 410 differential refractometer), and the sample and reference cells were held at 40 ºC. An Aminex HPX-87P column (300 mm x 7.8 mm i.d., 9-μm particle size) with a guard column cartridge (Bio-Rad Laboratories, Richmond, CA, U.S.A.) was used. Data were processed using the Waters Millennium 2.0 chromatographic data system.

Tartaric acid and malic acid: Individual acids were determined by HPLC as previously described by Esteban et al. [Esteban MA, Villanueva MJ and Lissarrague JR, 1999] The chromatograph employed was a Waters liquid chromatograph equipped with a Waters model 996 PDA detector. An Aminex HPX-87C cation exchange column (300 mm x 7.8 mm i.d., 9-μm particle size) was used, with a guard column cartridge (Bio-Rad Laboratories, Richmond, CA, U.S.A.). Data were processed using the Waters Millennium 2.0 chromatographic data system.

Relationships between different berry components.

Multilayer feedforward networks are often used for modeling complex relationships between the data sets. Deleting unimportant data components in the training sets could lead to smaller networks and reduced-size data vectors. The process of finding relevant data components is based on the concept of sensitivity analysis applied to a trained neural network. ANN models predict changes for certain combinations of input variables, detecting the most important influence in the output variables.

We have studied different analysis for detecting relathionships between berry weight or ºBrix and other grape components in the two irrigation treatments (T1=Irrigated and T2=non irrigated) during the ripening period.

In order to study the relationships between different variables it has been used neural networks models with a single hidden layer with 6 axons and a Tanhaxon transfer function and based on the momentum learning rule.

Study of the relationships between different variables and ºBrix in I y NI treatments

Analysis of the results

I	*Berry weight*	*Ph*	*Total acidity*	*ºBrix*	NI	*Berry weight*	*Ph*	*Total acidity*	*ºBrix*
	11.342	17.709	70.949	100.000		33.765	25.123	41.111	100.000
		22.712	77.288	100.000			41.958	58.042	100.000
	17.930	82.070		100.000		55.994	44.006		100.000
	14.877		85.123	100.000		37.859		62.141	100.000

Active performance of the analysis

I	*MSE*	*NMSE*	*r*	*%Error*	NI	*MSE*	*NMSE*	*r*	*%Error*
	0.03	0.01	0.99	5.76		0.004	0.01	0.99	6.66
	0.004	0.01	0.99	6.43		0.008	0.02	0.98	9.61
	0.008	0.03	0.98	8.67		0.005	0.01	0.99	6.72
	0.003	0.01	0.99	5.86		0.004	0.01	0.99	6.64

During the ripening period in berries of the cv. Tempranillo grape variety along a period of three years, it has been studied that the values of ºBrix in the two irrigated treatments are different. It has been analysed the importance that has the impact of some components (total acidity, pH and berry weight) on the ºBrix. Thus we observed that total acidity is the variable that influences most in the irrigated treatment with 70.9%, followed of pH with 17,7% and finally the berry weight with 11.3%. In the non-irrigated treatment occurs the same, reaching total acidity a value of 41,1%, however, the berry weight (33.7%) influences more than pH (25.1%). Analyzing variables two to two we verified that those models are the same in both treatments. Thus, the impact of the berry weight in the ºBrix in the irrigated treatment is less than in the non- irrigated treatment, this could be because of the concentration effect that takes place since the absolute values in both treatments are the same.

We have also analyzed Tartaric and Malic

I	*Berry weight*	*Tartaric*	*Malic*	*ºBrix*	NI	*Berry weight*	*Tartaric*	*Malic*	*ºBrix*
	8.556	31.008	60.436	100.000		40.110	14.112	45.778	100.000

Active performance of the analysis

I	*MSE*	*NMSE*	*r*	*%Error*	NI	*MSE*	*NMSE*	*r*	*%Error*
	0.003	0.001	0.99	5.22		0.003	0.01	0.99	6.04

We have analyzed the two most important acids in the grape because they determine the value of the total acidity. As it happens with the total acidity, both acids influence in the ºBrix value more than the berry weight in the irrigated treatment, whereas in the non- irrigated treatment this only happens with the malic acid and nor with the tartaric acid.

Study of the relationships between different variables and berry weight in I y NI treatments

Analysis of the results

I	*ºBrix*	*Ph*	*Total acidity*	*Berry weight*	NI	*ºBrix*	*Ph*	*Total acidity*	*Berry weight*
	29.960	15.411	54.629	100.000		60.653	28.628	10.719	100.000
	29.211	70.789		100.000		67.386	32.614		100.000
	37.080		62.920	100.000		76.970		23.030	100.000
		38.506	61.494	100.000			47.754	52.246	100.000

Active performance of the analysis

I	*MSE*	*NMSE*	*r*	*%Error*	NI	*MSE*	*NMSE*	*r*	*%Error*
	0.01	0.07	0.96	8.99		0.005	0.02	0.98	5.77
	0.02	0.08	0.94	10.4		0.005	0.02	0.98	5.88
	0.02	0.09	0.95	10.3		0.005	0.02	0.98	5.83
	0.03	0.12	0.93	10.9		0.02	0.11	0.93	11.08

It has been studied the importance of the impact of some variables (total acidity, pH and ºBrix) on the berry weight. Thus we observed that total acidity is the variable that influences most in the irrigated treatment with 54.6%, followed by ºBrix with 29.9% and finally pH with 15,4%. In the non-irrigated treatment ºBrix is the variable that influence the most in the berry weight with a value of 60.6%, then the pH (28.6%) and the total acidity (10.7%).

We have also analyzed Glucose, Fructose, Tartaric and Malic.

I	*Ph*	*Glucose*	*Fructose*	*Tartaric*	*Malic*	*Berry weight*
	22.645	18.624	33.515	10.830	14.387	100.000
		20.461	34.891	11.707	32.942	100.000
NI	*Ph*	*Glucosa*	*Fructosa*	*Tartárico*	*Málico*	*Berry weight*
	18.590	36.107	25.640	8.388	11.275	100.000
		41.808	24.284	14.115	19.793	100.000

Active performance of the analysis

I	*MSE*	*NMSE*	*r*	*%Error*
	0.01	0.05	0.97	7.93
NI	*MSE*	*NMSE*	*r*	*%Error*
	0.004	0.02	0.98	5.3

Glucose and fructose are the most important sugars in the grapes and they are the ones that determine mainly the ºBrix value. In the irrigated treatment pH is the variable that influences most in berry weight followed by fructose and glucose, although the amounts of the two sugars influence more than any other variable. However, in the non- irrigated treatment the impact of these two sugars is the highest.

Conclusion

The results with neural networks show that total acidity is the variable that influence most in ºBrix value in both treatments when the analysis has been total or with tartaric and malic acids, except in the case of tartaric acid in the non irrigated treatment. It is also shown that ºBrix value is the variable that influences most in the berry weight non irrigated treatment while total acidity is in the irrigated one.

These results provide that in both treatments, irrigated and non-irrigated vines, and during the different stages of the berry growth it is possible to establish significative relationships between the parameters studied. Glucose and fructose influence more in the berry weight than tartaric and malic acids.

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