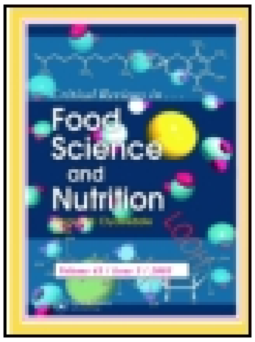

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A Critical Review on the Applications of Artificial Neural Networks in Winemaking Technology

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A CRITICAL REVIEW ON THE APPLICATIONS OF ARTIFICIAL NEURAL NETWORKS IN WINEMAKING TECHNOLOGY

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Abstract

Since their development in 1943, artificial neural networks were extended into applications in many fields. Last twenty years have brought their introduction into winery, where they were applied following four basic purposes: authenticity assurance systems, electronic sensory devices, production optimization methods, and artificial vision in image treatment tools, with successful and promising results. This work reviews the most significant approaches for neural networks in winemaking technologies with the aim of producing a clear and useful review document.

Keywords

Wine production; modelling; prediction; authenticity; optimization; electronic sensing

Artificial neural networks and its potential for winemaking applications

Artificial neural networks are mathematical tools which are parallel, distributed and adaptive data processing systems. They were inspired by the way biological neural systems process data, and learn from experience. They can find patterns among variables especially when their relationships are non-linear. They can be applied in multivariate regression problems (Mekanik et al., 2013), in classification tasks (Zhang, 2000), associative memorization (Liou and Lin, 2006), control systems (Chairez, 2013) or for simulation-forecasting purposes (Moldes et al. 2014).

The main idea trying to reproduce brain abilities lies on computers being traditionally designed for high-level tasks. This implies that they can affordably make calculations or reasoning, for example, and generally anything that can be achieved by processing symbols. They do not succeed in the same way in low-level duties like pattern recognition or control, fields where nature have found a better approach through self-organizing processing, which rises from interactions of several single elements. Therefore, artificial neural networks were developed focusing into reproducing this capabilities.

Neural networks, in virtue of their parallel distributed structure and learning capabilities (and therefore, generalization), present some interesting properties (Haykin, 2009). Generalization refers to being able to produce acceptable outputs for a specific set of inputs not used in learning and consequently unknown for the network. Generalizing can be understood as a good nonlinear interpolation of data. It is what makes neural networks a versatile tool that can find approximate solutions for many situations, especially when they are complex problems and there is no satisfying theoretical model to apply.

By means of its built-in plasticity, neural networks can adapt to changes in their environment. Such a property make them really fault tolerant (*i.e.*, a malfunction in one of its neurodes), at least when networks are implemented in hardware form. In this way, neural networks performance will decay softly instead of a sudden stop working. It must be taken into account that actually most works with neural networks are easily implemented through virtual simulations in standard hardware. But adaptation implies too that networks can evolve to confront environment changes, and, then, a network trained in a specific background can again be trained with new conditions.

Learning is operated by self-organization. Based on examples, inputs are mapped with outputs in what is commonly known as a training stage, which remind us of a typical requisite of neural models: an adequate, representative of the problem database of examples is needed. Even when it is available, it is not possible to assure that a neural model would be able to find the proper outputs for all the possible input cases, neither the optimal solution for everyone (but it might be a sufficiently good one).

Neural networks create its own representation of the information they deal with, in its own (and distributed) way. This has some undesirable implications, because it provides neural network models with a strong black-box character, in the sense there is not an easy method to recover such a model in a human understandable manner for interpretation and so we can only access to the outputs related with their inputs. Some techniques have been developed in order to extract some knowledge from neural networks (Boger and Guterman, 1997; Kemp et al., 2007).

There is a last unpleasant feature in neural networks modelling, overfitting, which implies a lost in generalization power. As a result, the network is not generalizing but memorizing the dataset instead, including inner noise. Occurs when inputs-outputs mapping fails with cases that were not present in the learning stage and it is typical to happen when learning takes too much epochs to fulfil, or when the model is built with too much nodes and then depends on too many parameters. Overfitting can be somewhat avoided following recommendations, but, once again, it is not possible to assure when a network is overfitting until it is manifestly obvious. A cross validation with cases not present in learning would result useful to determine when fitting is near an optimum point, and is usually applied in most of neural models like multilayer perceptrons. The key point is to adequately dimension the network size in concordance with the complexity of the problem (Martínez and Sanz, 2001). Early-stopping techniques have been developed as they avoid overfitting by limiting the number of parameters of the network without changing its architecture. In this sense, to reduce the number of parameters a technique like Principal Components Analysis (PCA) or similar approach can be applied for diminishing data dimensionality. Indeed, most of times just screening that error is kept in modelling under a consensual value: 0.5% or 0.1% is usually enough.

Networks are built with single units usually so-called nodes or neurons, (even sometimes *neurodes*, from *neuron* and *node* fusion) which are organized in levels of neurons commonly known as layers. The first one is the input layer, the following the hidden or intermediate layers, and the last the output layer. Input layer picks up relevant data for the model and output layer produces estimations or categories based on input data.

Inner structure of a neuron is composed of three functions, and their properties influence in the behaviour of the network, even though there are other factors that determine the way a neural network works, as discussed below. The first one is the propagation rule, depicted in equation 1 in its typical form, where w_{ij} stands for the weight of the connection of neurons i and j, and x_j the value of the previous neuron j (or just an input), and modified by a bias b. It collects and performs a weighted sum of input signals that enter the neuron. Weights in this case represent intensity of every single input for a specific instant. Its output is then operated by the second function, the activation or transfer function showed in equation 2. Several activation functions are commonly used, standing out sigmoidal or step functions. It resolves whether the neuron will fire or not according a threshold (Russel and Norvig, 2010). At the end is the output function, which takes activation signal and produces the final output value of the neuron, being that it is usually and identity of the activation value as presented in equation 3. Figure 1 depicts a scheme of such a neuron for an easier understanding.

Equation 1 $$P_i(t) = \sum w_{ij} x_j + b$$

Equation 2 $$A_i(t) = f_i(P(t))$$

Equation 3 $$Y_i(t) = A_i(t) = f_i(P(t))$$

Activation function works as an analogy of the way biological neurons receive several inputs from other neurons. A node is connected with more nodes from the previous layer and is connected to nodes from the next level. When working, signals from nodes from the previous level are collected and processed by the activation function. This is made according to the relative weights of those signals. Then, activation function establishes if the sum of the whole set (provided by the propagation rule) is strong enough to fire the neuron, so the signal continues to the next layer of the network controlled by the output function. The value produced here can be incorporated as an input into another neuron, and, in this way, neurons are interconnected from the input layer to the output, as showed in figure 2.

Weights have a role in the connection, as they establish the relative strength of the signal form a particular neuron with respect to others. With different weights the network will produce different results. Therefore, building the proper neural network has much to do with finding proper values for weights. The learning process accomplishes this through training. Training is an iterative process where weights are adjusted to obtain sufficiently good outputs. It strongly depends on the learning algorithm, which typically modifies weights after an iterative cycle (some authors refer them as epochs) according to how different are the outputs produced in this cycle to theoretically correct values. Learning algorithms are diverse, with different features in order to perform better in different circumstances. After training, a generalization test is usually performed according several techniques, such as cross-validation.

The interest of neural networks is that they can simulate complex problems to produce accurate estimations, particularly those where the relationships among variables are unknown or non-linear. With a proper dataset, that means, representative of the phenomenon, and training, it is theoretically possible to approximate every function with a neural network (Hornik et al., 1989).

It must be noticed that the way networks built their own model usually does not help at all in understanding the simulated system, because of their self-organizing black-box modelling.

Learning can be implemented in four ways (see figure 3 for several examples). First, we have supervised learning, which lies on giving a dataset, composed of several parameters and their corresponding output values. Therefore, it adjusts its weights iteratively considering previous deviations, in order to estimate the outputs. It must be emphasized that an external agent supplies the correct answers, and this is where the *supervised* term comes from. Multilayer Perceptrons (MLP) are the paradigmatic architecture of supervised learning (Moldes et al., 2015). They are composed of several layers of neurons, where information spreads feed-forward from inputs to outputs through several layers of neurons, and, then, a backpropagation algorithm connects back with the network.

Unsupervised learning is also possible. In this occasion, there is no external agent, and networks produce estimations for datasets without knowledge of which are the desirable outputs. For this reason, this is also known as self-organizing learning, because the network recognizes inner properties and bounds of the dataset to uncover them. Kohonen Self-Organizing Maps (SOM) are popular unsupervised networks, commonly applied in classification tasks (Martínez and Sanz, 2001; Kohonen, 1982). They have two layers, one for inputs and other for competition (see figure 4). In the competition layer similar inputs are depicted close to one another. The term competition refers to the weight adjustment occurring in this layer, as the neuron which fits better with an input wins and modify surrounding neurons that evolve to be similar to the winner.

As closer neurons became more alike, at the end a map of features grouping related inputs is obtained.

Hybrid learning can be implemented as well, usually with both kinds of learning occurring separately in different layers. Radial Basis Function networks (RBF) are similar to backpropagation networks but differ in the Behaviour of the hidden layer, where activation relies on radial basis functions (see figure 4). Euclidean distance between weights and inputs is calculated in a Kohonen SOM fashion and only cause neuron activation when it is similar to a specific value known as center (Martínez and Sanz, 2001; Schwenker et al., 2001). As a result, these networks have a faster learning.

In a kind of midpoint between supervised and unsupervised learning lies reinforcement learning. Even though it uses information about estimation errors, the real desirable output is unknown and, therefore, external agent just indicates to the network if its performance is good or bad, a reward or punishment mechanic where the learner focuses on maximize reward (Tesauro, 1995).

McCulloch and Pitts are credited for the first work in neural networks in 1943 (McCulloch and Pitts, 1943). Hebb would introduce the first rule for learning six years after that (Hebb, 1949). Already in 50s, a hardware neural network would be developed by Minsky and Papert (1988). Rosenblatt would design the modern perceptron, although at the time it was considered just a mathematical work (Rosenblatt, 1958). In 1962, Hoff and Widrow’s MADALINE would become the first neural network successfully applied into a real world problem (Baikal and Yildirim, 2013). As a consequence of the subsequent work of Minsky and

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Papert (1988), criticizing perceptrons and their power to solve problems of interest, research in neural networks suffered a slowdown that would last until 80s, when Rumelhart and colleagues developed the backpropagation algorithm that would solve known training issues and mark the revival of neural networks research. Since then, according to their multidisciplinary feature, neural networks have been applied successfully in a whole lot of fields (Valdés et al., 2012; Nemati et al., 2013; Asimakopoulou et al., 2013; Meena et al., 2013; Maurelli et al., 1998; Acioli et al., 1999; Nemati et al., 2014).

That leads us to winemaking, a complex process where multiple variables are involved and where it is usual that the enhancement of a parameter implies low quality for other one. Besides, wineries commonly have great bulks of data from past vintages that remains of no use. Artificial neural networks, in virtue of their classification capabilities can be of interest for optimization tasks and have a potential for learning from those datasets. The identity of wines has a huge economic impact and so is an incentive for fraudulent behaviors. Discrimination of clue signatures of wines into their origins can be achieved with neural networks. Finally, the elaboration of devices for winery applications was achieved. This review work focuses on the applications of artificial neural networks in winemaking for the last twenty years. During this time, neural networks have been mainly implemented for authenticity insurance systems, for the development of sensory devices biologically inspired as alternative analytical methods, and for optimization of production parameters, but also artificial vision technology based on them was developed for ampelographic uses.

Imaging treatment in vine cultivars identification

Visual examination of grapevines is traditionally employed in harvesting decisions. Considering biases and errors associated with human condition, there is a role for artificial vision to take their place, and the overwhelming presence of digital cameras everywhere just boost this process. Artificial vision is one of the main fields where the pattern recognition feature of artificial neural networks is used (Chtioui et al., 1997). Viticulture and ampelography can take advantage of this for ripeness evaluation or varietal identification of cultivars from several vine organs, like seeds of leaves.

Some particular grape varieties are considered especially suitable for obtaining wines with specific qualities. A fast, easy and cheap method for variety recognition is desirable since a wine-making point of view, as long as more than 10,000 varieties are known of *Vitis vinifera* (*i.e.*, more than 1,000 indigenous varieties are known in Galicia, a region with just 26,000 ha of vine cultivation (Robinson, 2006)). We have a legacy of several names for the same varieties around the world that evidence that identification has historically been a serious trouble. As an example, vine nurseries of the New World are known for traditional mistaken identification of their plant material in the past, with considerable inconvenient for producers (Robinson, 2006).

Briefly, an artificial vision device needs to process the image in order to extract features, like specific shapes or ranges of color, which then can be classified according to trained patterns. Recent approaches on this topic are summarized in table 1. Mancuso and his colleagues developed systems based on the recognition of specific foliar features that can separate samples into different cultivars. Their work from 1998 relied on multilayer perceptrons trained with backpropagation algorithm, and resulted in a fast, solvent, cheaper, alternative biometric method

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for genotype classification of vine leaves contours (Mancuso et al., 1998). A similar classifier was developed, based on Elliptic Fourier Analysis (EFA) descriptors, a powerful method for image description, with promising results that opened a path to study varietal characteristics that might not be detected with conventional methods (Mancuso, 1999). The EFA approach was resumed in a work with Kohonen SOM instead of MLP. Aside of being a fast, cheap method too, SOM offered an easier interpretation of the model (Mancuso, 2001).

Avila et al. (2013) proposed a system to process pictures of grape seeds useful to determine ripening of vintages. A multilayer perceptron, trained according to Bayesian regularization algorithm, processes texture descriptors to segment shadows in complex images of seeds. Descriptors are obtained through the application of several invariant models to lightning. Considering ripening, the determination of sugar content of grapes for Port wines through hyperspectral images classified by neural networks was suggested (Gomes et al., 2014). Hyperspectral images provide spatial and spectral information by integrating spectroscopy and digital imaging techniques. The system takes data in reflectance mode, in other words, the information about how objects absorb or reflect different wavelengths of light. The advantage of this technique relies on no contact with the grapes is required and also several points are analyzed at once. Multilayer perceptrons trained with the Levenberg-Marquardt algorithm are applied to classify input profiles according sugar content. Since good results were obtained, the method offers a cheaper, consistent, objective technique that can be applied in inspection, evaluation or for measurement purposes.

Prosecution of authenticity frauds

Wine adulteration is historically a common practice elsewhere. It is well known that, in ancient Greece and Rome, wine was consumed diluted with water (Gozzioni Giacosa, 1994; Apuleius, 2010). Such behaviors would last for centuries, as wine usually was a safer drink than water at the time. In 18th century in Bordeaux, adulteration practices prospered and led to what was so-called a *travail à l'anglaise,* which consisted in mixing a wine with a cheaper one, looking for a product to satisfy British tastes (Le Gars and Roudié, 1996). At the time, in Porto, wines where added with brandy in a preparation that later would result into Port wines as we know them nowadays. Fraud was also committed when the costumers were absolutely unaware of those tricks (Robinson, 2006).

Nowadays many popular trademarks in winery refer to geographical places. Not only quality but also commercial value for wines is often linked to its region of production (several countries have developed controlled appellations, public trademarks based on the French *appellation contrôlée* system of quality marks (Robinson, 2006)). It must be appointed that many productions consist in relative smaller areas of limited production. That is the reason why authenticity is a key for companies that sell these certified products, as origin is one of their main differential attributes, which is reflected in the final price in any case. It is clear that a demand for authenticity tools exists, and that neural networks were extensively employed in applications for authenticity elucidation.

The basis for authenticity tools based on neural networks lies on their capabilities for pattern recognition and then classification of cases according to selected rules, which let us to determine with accuracy whether a new case corresponds with a category or not. Categories may be cultivars, regions of production, and vintages of a specific year or whatever as long as the neural model can find reliable patterns. Table 2 contains the main approaches in this field in the last decades. Briefly, they consist in software applications for data analysis, complete analytical devices, or the foundations for a database construction.

Aires de Sousa published in 1996 a work where multilayer perceptrons were applied to build wine classification tools according to controlled appellations or variety (Aires de Sousa, 1996). Chemical composition profiles of anthocyanin or aminoacids were inputs of the neural models, and backpropagation algorithm controlled the training process. This early approach was back then considered a promising tool for wine classification. Classification is a task that Kohonen SOM commonly performs better. Aires de Sousa and collaborators applied them to separate wines of different varieties, but also to check whether is possible to distinguish between wines that pass or not through malolactic fermentation (Cabrita et al., 2012). Inputs were based on polyphenol contents obtained via reversed phase liquid chromatography with diode array detection.

UV-VIS and NIR spectral fingerprint of wines were employed for the development of classifiers built with multilayer perceptrons and neural fuzzy models. Gaeta et al. (1998) preprocessed spectra to look for the most significant absorbance peaks to feed the neural models. Fuzzy models exhibited better performance than multilayer perceptrons. Marengo et al. (2001) applied a Kohonen SOM to build a classification tool that segregates wines according to their production zone and vintage year. Inputs for the system were solid-phase microextraction coupled with gas

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chromatography-mass spectrometry (SPME GC-MS) data peaks corresponding with volatile compounds of samples.

Again, Kohonen SOMs were employed, this time by Frías et al. (2002) for Canary Islands wines. Their work begins with the assumption soil composition determines metal content in crops, and, because of this, crops reflect the particular composition of a region. Their neural model, fed with metal composition of wine samples, can properly classify wines according to island of origin and ripening degree of grapes. A multilayer perceptron trained with backpropagation was thereafter developed with fewer input variables that however improve classification rate. Similar results would be obtained in a later approach (Diaz et al., 2003). The metal concentration proposal returned in the work by Álvarez et al. (2007). They argue that minerals, because of their correlation with soil and grape variety, are the best place to perform a differentiation based in origin, and it can be accomplished using major, trace or ultra-trace elements. Their work consisted in the development of a classification method for fino wines of different DOs. Mineral content was obtained via inductive coupled plasma optical emission spectrometry, and the more discriminant ones were selected to feed a multilayer perceptron trained with backpropagation algorithm.

The work by Pérez-Magariño et al. (2004) displayed a neural network method that can distinguish wines from eight different origins elaborated with very similar grapes. It consists on a multilayer perceptron trained according the Guterman-Boger algorithm. It replaces non-significant neurons with biases that act in the same way to save computational power. They calculated causal indexes, since they can give information about the influence of a variable for a data set. The work by Pazourek et al. (2005) consists in a multilayer perceptron that processes fingerprints of a wine obtained through solid phase extraction electrophoresis. As a result, a classifier is obtained with the capability to separate samples according its precedence. The network was trained with a combination of backpropagation and quick propagation algorithms.

Considering meteorological and edaphic conditions leave a characteristic fingerprint in grape phenotype, Masoum et al. (2006) elaborated a neural design for a classifier to separate wines. Phenolic compounds are vine secondary metabolites, which production depends of the growing conditions that are present in wines. To feed up the model, a Learning Vector Quantization neural network (LVQ), two-dimensional NMR spectra polyphenol profiles were obtained and preprocessed through orthogonal signal correction. Obtained model can distinguish grapes variety, vintage year and soil of origin of wine samples. Phenolic compounds were also used as classification patterns in the approach of (Beltrán et al., 2006). This group obtained HPLC-DAD chromatograms of those chemicals and then applied several feature extraction techniques because of the inadequately high data dimension of the dataset, in order to apply several classifier techniques. One of them consisted in the development of a Probabilistic Neural Network. Combined with wavelet transform of the resampled chromatogram with the computation of the correlation coefficients in the time domain as feature extraction technique, it reaches the highest classification rate of their whole set.

Kruzlicova et al. (2009) proposed their own authenticity evaluator system based on artificial neural networks. It works with gas chromatography with mass spectrometric detection data for pattern recognition, and is able to classify wine samples into different variety, location and year of production. Classifiers are multilayer perceptrons training with quick propagation or quasi-Newton propagation algorithms. They found that a model developed after a reduction of input variables performs better than other based on the complete set of inputs. The group of professor Mejuto built a multilayer perceptron trained with backpropagation, which can classify wines from Vinhos Verdes controlled appellations according to three possible winemaking processes (Astray et al., 2010). Inputs include chemical parameters and production data like the clarification method employed.

Martelo Vidal and Vázquez built classifiers for wines according their controlled appellations of precedence and the grape variety in a two parts work (Martelo-Vidal and Vázquez, 2014a; Martelo-Vidal and Vázquez, 2014b). Analytical data for inputs was obtained in both cases from UV VIS NIR spectra, and fed multilayer perceptrons trained through Bayesian regularization. So, they could perform fast classifications for controlled appellations segregation, even in subregions of Rías Baixas. It must be taking into account that controlled appellations O have restrictive requisites related to geographical origin and cultural techniques that effectively implies great similarity among their wines. Also, their model worked well with grape varieties.

In their work, Šelih et al. (2014) analyzed the elemental composition of several Slovenian wines. Looking for an authenticity tool for origin evaluation, they tried a principal component analysis that somewhat fail. So they proceed with a neural chemometrics technique, a Counterpropagation Neural Network (CPNN), and they achieved an acceptable classification of white wines into main production regions, and even sub-region for some samples. Inputs for the model derived from elemental analysis of samples through inductively coupled plasma mass spectrometry and optical emission. Hosu and partners published a work where developed a series of classifiers based on Probabilistic Neural Networks (PNN) to separate wines according to authenticity relevant groups (Hosu et al., 2014). Their models are built with UV-VIS spectrophotometric measurements for polyphenol determination in samples. The approach by (Bednárová et al. (2013) considered that an authenticity tool might be built around typical oenological variables of regular obtainment in wineries. Indexes like alcoholic grade, density or pH should be more desirable for producers than other sophisticated proposals that can be found in literature. They developed classifiers according to several data analysis techniques, including neural network modelling. They found they could successfully classify wines depending on variety and geographical origin. Their models were multilayer perceptrons trained with the Broyden-Fletcher-Goldfarb-Shanno algorithm.

Analytical methods and sensory devices for fingerprinting quality control

Last decade has seen improved development of the so-called electronic noses and tongues (depending on the analyte, whether it is a liquid or a gas). They consist of several sensors coupled that send a complex signal to a processing unit. Sensors are of low selectivity for a wider measurement range, and then a computational system processes the signal in order to offer an interpretation of useful data clean of noise. As sensor arrays signals might be composed of a huge amount of data, data pretreatment is usually a must for reduction in complexity and increasing on processing speed. Electronic noses and tongues are analytical tools composed of two main elements, as it is pictured in figure 5. The first one is the sensory device itself, commonly a group of sensors coupled for analytical power enhancement. Three kinds of sensors are the usual technology for liquid samples, being potentiometric, voltammetric and enzymatic biosensors (in the case of bioelectronics devices), but also impedimetric and amperometric among other exist (Zeravik et al., 2009). On the other side, electronic noses are commonly built around chemoresistors, gravimetric sensors, or optical devices (Röck et al., 2008). The second element is the mathematical processing unit needed to make sensor data comprehensible and meaningful, which is usually achieved by chemometrics. Through mathematical processing, information can be obtained in two ways. First, by multivariate calibration, sensor signals can be related with analyte concentrations. Second, samples can be classified into different groups according their signal profiles. In both approximations, artificial neural networks have a role, as illustrated by the references showed in table 3.

Analytical methods, on the other hand, employ neural networks in a different way. Looking for easy-to-apply, non-destructive techniques artificial neural networks can link specific signal profiles with a concrete chemical composition. This means that once we have a sufficiently large database for training, obtained with traditional analytical procedures, an artificial neural network based technique can be employed for a chemical composition analysis less time-consuming. All of these approaches, analytical techniques or electronic devices, both have in common the development of fingerprint control tools. More recent ones are summarized in table 3.

The electronic nose by Yamazaki and colleagues applies a time delay neural network, trained with a modified Levenberg-Marquardt algorithm, to correspond the output of an array of chemoresistor sensors with the vintage of the wine samples. This way, a classifier is obtained for vintages of wines that performs better than similar systems based on multilayer perceptrons (Yamazaki and Ludemir, 2002). This work was a first step that would later be continued (Ludemir and Yamazaki, 2003).

Penza and Cassano (2004a) developed an antifraud device based on an electronic nose. Powered by mixtures-of-experts arranged neural networks trained with backpropagation, it can recognize adulteration of wines by ethanol, methanol or other wines addition. Sensory array is composed of chemoresistive sensors. Similar sensor array was implemented to develop another electronic nose where a multilayer perceptron classified sensory output profiles with the chemical composition of the sample after training with backpropagation algorithm (Penza and Cassano, 2004b). As a result, a portable device suitable for in situ or online measurement was developed. Riul Jr. et al. (2004) built and electronic tongue instead, but its fundamentals are similar. Again, the chemical fingerprint of the samples is applied to a multilayer perceptron trained with different training algorithms to classify impedance signal of the sensor array with the identity of the samples. The method developed by Tiefenbrunner et al. (2009), referred as an artificial wine taster, acts as an electronic nose. It is a classifier that can recognize a specific must and a wine’s particular yeast strain. Inputs for the neural model, a multilayer perceptron, are obtained by solid-phase microextraction with gas chromatography–mass spectrometry determination of the headspace (Headspace-SPME-GCMS).

Cetó et al. (2012a) developed another electronic tongue for polyphenol analysis in wines. Designers faced the task of processing the complex analogic signal produced by their array of amperometric sensors and relate it with polyphenol content. So, the obtained voltammograms have been first preprocessed by means of discrete wavelet transform. Then, a multilayer perceptron trained with the Bayesian regularization algorithm finally managed signal. Network is kind of complex, as different propagation functions were implemented in hidden and output layer. The whole system is complemented by PCA calculations in parallel, which can process the same datasets for polyphenol discrimination. This way, they offered an alternative polyphenol analytical system to traditional methods.

With the same purpose of determining polyphenol content in wine this group tried a different device, a bioelectronic tongue, which essentially is an electronic tongue with enzymatic sensor arrays. Voltammetric signal was preprocessed with the Fast Fourier Transform (FFT) before feeding a multilayer perceptron for training according the Bayesian regularization algorithm. This neural model can predict the Folin-Ciocalteu and UV polyphenol indexes of a wine, but is complemented with a parallel PCA-multilayer perceptron classifier that can discriminate among the studied polyphenols. This last one applies backpropagation algorithm in training (Cetó et al., 2012b). Other approaches were developed by Cetó et al. (2014), *i.e.* an electronic tongue trained to classify cava wines according to their ageing times. The device has several voltammetric sensors and applies a multilayer perceptron to estimate dryness of a sample. According to authors, a more recent work with an electronic tongue represents the first attempt that successfully reproduces scores that a sensory panel gives to a wine (Cetó et al., 2015). With a voltammetric sensor array, they reproduced the tasting perception of a group of sommeliers. Sensor signal was preprocesed with Fast Fourier Transform compression and fed a multilayer perceptron trained with backpropagation algorithm. The electronic nose by Aguilera et al. (2012) is a classifier for wines. Partial Least Squares (PLS) and Independent Component Analysis (ICA)

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were applied as dimensionality reduction. Assayed models are based in a backpropagation multilayer perceptron and in Probabilistic Neural Networks (PNN). Sensor array is composed of chemoresistive sensors.

Fu et al. (2012) developed an electronic nose for classification of samples of several products, including wines. It is powered by a chaotic neural network known as KIII, a massively parallel architecture of several layers with positive and negative feedback loops (Fu et al., 2005). The role of the neural model is to act as an associative memory to store previous trained patterns, to be recovered when defective patterns are faced. The training algorithm is a combination of Hebbian reinforcement learning and global habituation rules. The device employs PCA for dimensionality reduction, finding that seven principal components offer a good solution in the trade-off between calculations time and classification success rate. Electronic nose was built with Taguchi gas sensors, and the sampling process works at room temperature, an advantage over most of similar devices. The work by Macías et al. (2013) is focused in developing a low-cost electronic nose prototype. They employed a microcontroller, two micropumps, two electrovalves and a chamber with Taguchi gas sensors, with an approximate final cost of 200$. The device employs a multilayer perceptron for classification purposes, and was tested with several alcohol aqueous solutions as synthetic wine samples. This electronic nose can successfully classify samples in different categories according to their concentration, being comparable with other commercial devices but cheaper. Still susceptible of improvement (Macías et al., 2014), it may be applied to real wine samples.

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Hosu and colleagues, with multilayer perceptrons trained with the quasi-Newton Levenberg-Marquardt algorithm, carried out models for antioxidant activity prediction of wines (Hosu et al., 2014). Those models are fed with four UV/VIS spectrophotometric indexes related with the antioxidant activity of a wine. Their models work well with any combination of the input indexes, which has a potential for saving time and costs. Martelo and Vázquez (2015) were working in a neural method for fast quantification of several wine compounds, like ethanol or tartaric acid, using UV-VIS-NIR spectroscopy as input data. Based in multilayer perceptrons fed with the spectral data, produces estimations of the chemical content of the sample. A PLS pretreatment has been applied in order to reduce dimensionality of the inputs. This system has proven good results using chemical standards, and needs to be test with real wine samples.

Reliability of electronic devices makes them suitable for online, real-time measurements according to Lozano et al. (2015). Their work proposes an electronic nose for wine evolution monitoring. The system is fully automated and is able to detect changes in the aroma profile for months, which can be applied into fermentation or preservation of grape juices when winemaking or storage, warning about off-odors in time for corrections. A probabilistic neural network classifies analytical profiles according to its aging.

Optimization and decision making in wine production

Mathematical modelling is an effective approach to understand the influences of the factors involved in a productive process. A predictive model offers the possibility to simulate the result of production choices without having to confront undesired economic consequences and so, doing decision making easier. Artificial neural networks, as a tool for non-linear multivariate modelling, can be employed for developing models based on a few critical values, with enough accuracy that an operator can take corrective decisions in time for saving a batch. On the other hand, introducing changes in a process does not lack of risks of losing investments. In this situation, a predictive model can offer a pretty precise overview of the consequences of such changes. Information tracking and quality evaluation of processes implemented considering neural networks offer an opportunity for solving problems in advance. Those applications might be implemented independently of the data collection technologies, and literature has examples for several spectroscopy techniques, specific sensor signals or traditional winery variables, as demonstrated in table 4.

Vlassides et al. (2001) proposal consist of taking advantage of the records of past productions to improve future fermentations. They considered that all the data produced in years in a winery could be fully employed to optimize wine production. Their system, powered by MLP trained with the backpropagation algorithm, allows producers to use historical data of the winery, and relate it with critical parameters of the production, a method that may also be exported to other fermentative processes. From features of the variety and the intended processing, the model can predict kinetics and sensory properties of the final product.

To obtain certain desirable characteristics might be achieved by monovarietal wines blending. But the process is actually more complex than it seems as an enhancement in a specific characteristic might degrade quality of other one. (Ferrier and Block, 2001) developed a neural system that optimize blends and let the users achieve final products much closer to the desire wine. Their method is based in backpropagation networks trained with the Broyden-Fletcher-

Goldfarb-Shanno algorithm. About blending, Ren and Ii (2006) have a different approach. It must be notice that winemaking in China is extremely unalike than the Western productions. Traditionally, there is no difference among wine and other alcoholic beverages, and it might consist on mixtures of wine with other juices different from grape or other additives, rather than the simpler fermented grape must (Robinson, 2006). Their work consist in the development of a wine body's database with a management system that depends on a backpropagation network for autoblending of wines. The neural model extracts connotative information from the samples used to build the database, so the management system can mix a blend of several liquors in order to fit with a standard. A sample of the final blend is checked to test its quality to establish whether it must go back to the blending system or whether it is ready for packaging.

Predictive capabilities of neural networks were taken advantage by Urtubia and colleagues (2012). They have developed a forecasting model to detect in advance abnormal behaviors of fermentations, so corrective actuations can be applied. Just three variables input a multilayer perceptron trained with backpropagation algorithm that achieves an early detection of troubling batches up to 72 hours (Román et al., 2011). Similar approach would later lead to another detection system, with a multilayer perceptron trained with backpropagation with gradient descent algorithm (Urtubia et al., 2012).

A quality control system based on radio frequency identification (RFID) which provides warning to the operator when something abnormal happens but also gives quality information to the costumers, have been designed and implemented by (Wang et al., 2012). The system applies to winemaking as to distribution. Consists in two parts, the tracking and the evaluation systems, and can provide critical information of every step of the productive method, which allows decision making less dependent on traditional, subjective means. A perceptron trained through the Delta rule is part of the evaluation system, based on the *k*-nearest algorithm. Quality assurance of wines may be achieved through Fourier Transform Infrared Spectroscopy measurements (FTIR), as it requires minimal or no sample preparation at all, and so, it is a non-destructive technique. Agatonovic-Kustrin *et al*. (2013) developed a predictive method that applies neural networks, specifically a multilayer perceptron trained with backpropagation algorithm, to correlate those spectra with the values of typical quality indexes like total phenolic content, volatile acidity, pH or alcohol content. As a result, the model can, from spectral data, predict the corresponding value of such indexes.

Considering quality, tartaric acid precipitation is an important issue for commercial life of wine, as the presence on the bottom of bottles of tiny crystals invites consumers to doubt about the product or the production process. Taking this into account, (Malacarne et al., 2013) developed predictive models of instability for wines based on artificial neural networks. They used FTIR to obtain spectra from several samples of red, rosé and white wines. Then a multilayer perceptron, trained with backpropagation algorithm, processed data to build successful models of tartaric acid precipitation in bottle.

Lees are by-products of wine production rich in polyphenols that can be, for example, added into wines for structure correction or color stabilization. The obtaining process implies ultrasound-assisted extraction, an interesting method because of its high efficiency at relatively low cost and low environmental impact due to low consumption of solvents. Tao et al. (2014)

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proposed a neural approach that models the extraction process, a multilayer perceptron trained with backpropagation algorithm, so a genetic algorithms method can optimize the process.

Research gaps and future prospects to be addressed

This work tried to summarize the main applications of neural networks in winemaking technologies. Due to their generalization capability, derived from its learning feature, artificial neural networks can be successfully employed to solve problems involving predictive modelling and classification task, as demonstrated in references. Main approaches can be classified into four categories: i) image treatment; ii) authenticity tools; iii) new analytical procedures and devices; and iv) decision making in production. Many of the works reviewed might be easily adapted for other production processes, most notably those based on fermentations.

Datasets needed for learning needs to be representative of the case of study, what implies they have to be really specific for the situation. To obtain such data depends on traditional methods, so neural approaches are just faster, cheaper, maybe more convenient, but not absolute substitutes. Also, if the dataset becomes too large, problems with generalization are expected and dimensionality reduction techniques become in need. Hence, low or none at all knowledge extraction can be expected of a neural network implementation.

Wineries usually produce data that can be applied into a neural network solution, and this solution can be re-trained with newer data whenever needed. Many references notice their neural approaches to need no sample preparation and to be non-destructive, being commonly faster and cheaper than traditional methods. This way, even when alternatives exist with no need of giving up to knowledge extraction, like linear or partial least squares discriminant analysis, neural

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networks are a simpler solution whether this can be neglected. Even though many references exhibited just a framework instead of a final design for their proposals, improved instalments are supposed to come. Their promising results open an opportunity to develop user-friendly customizable do-it-yourself applications for neural network. Such tools would need few technical knowledge of the operator but would offer a powerful tool for supporting decision making or accelerating analytical processes, fed by self-obtained winery data.

Finally, electronic devices that can apply machine sensing in production can avoid human biases in perception, together with a potential for in situ, online or even portable measurements. Cheaper devices will help in a deeper market acceptance.

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Table 1. Artificial vision in ampelography

Approach	**Architecture**	**Inputs**	**Reference**
A classifier for vine genotype through leaf identification	MLP 15-10-15	Ampelographic foliar descriptors	(Mancuso et al., 1998)
A classifier for vine genotype through leaf identification through Elliptic Fourier Analysis	MLP 15-10-15	EFA descriptors of leave contours	(Mancuso, 1999)
A classifier for vine genotype through leaf identification through Elliptic Fourier Analysis, obtained with unsupervised learning	Kohonen SOM	EFA descriptors of leave contours	(Mancuso, 2001)
An artificial vision tool for separation of shadow areas of seed images for ripening evaluation	MLP	9 texture descriptors	(Avila et al., 2013)
Classifiers for hyperspectral profiles of grapes in order to determine sugar content	MLP	Some principal components	(Gomes et al., 2014)

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Table 2. Authenticity tools

Approach	**Architecture**	**Inputs**	**Reference**
A classification tool to discriminate wines according two different DOC. Another tool for wine classification according to variety	MLP 16-2-2	Anthocyanin composition percentages and a bias	(Aires de Sousa, 1996)
	MLP 23-8-8	Amino acid composition data and a bias	
A tool for classification of wines based on UV-VIS-NIR spectra fingerprints	Neural Fuzzy Model	Several specific absorption spectra wavelengths	(Gaeta et al., 1998)
Coupling gas chromatography with mass spectrometry of volatile compounds they built a classification tool for wines according origin and vintage	Kohonen SOM 7x7	35 peaks corresponding to volatile compounds of the sample	(Marengo et al., 2001)
Two classification tools based on metal content profiles of samples were developed. They can separate wines into their DO	Kohonen SOM 4x4	11 metal contents	(Frías et al., 2002)
	MLP 3-2-3	Mn, Sr & Rb content	

With metal content profiles, they developed classification tools which is able to segregate wines according their DO	Kohonen SOM 6x6	11 metal contents	(Diaz et al., 2003)
	MLP 4-5-4	Li, Sr, Mg & Mn content	
A classification tool for wines based on several, typical winemaking variables	MLP 7-4-3	Fe, Cu, Ca, total anthocyanins, total polyphenols, titratable acidity and total SO2 content	(Pérez-Magariño et al., 2004)
A classification tool that distinguishes vintages and cultivars from electrophoregraphic polyphenol fingerprints	MLP	Concentration of *cis* ant *trans* reverastrol, and 5 electropherogram peaks (the most intensive for white and red wines separately)	(Pazourek et al., 2005)
A classification tool based on NMR polyphenol profiles which can distinguish vintage, variety and soil of origin	LVQ 2.1	Polyphenol NMR spectra	(Masoum et al., 2006)
A classification method for wines according to vintage, valley and	PNN	Phenolic chromatographic data	(Beltrán et al.,

vineyard of origin consisting in a combination of a feature extraction method with a neural model as classifier			2006)
A classification method which discriminates between two different DO from metal content profiles	MLP 8-2-2	K, Sr, P, Na, Al, Fe, Mg and Mn content (most discriminating of 12 metals)	(Álvarez et al., 2007)
Classification tools to separate wines according to variety, vintage or producer from gas chromatographic with mass spectrometric detection profiles	MLP 7-3-3	7 volatile compound concentrations	(Kruzlicova et al., 2009)
	MLP 7-3-3	7 volatile compound concentrations	
	MLP 17-11-5	17 Volatile compound concentrations	
A classifier based on physicochemical and oenological data for Vinhos Verdes	MLP	Vintage, Clarification technique, pH, Absorbance at 420, at 520 and at 620, Tonality and color	(Astray et al., 2010)
A classifier to separate wines according variety and whether malolactic fermentation was	Kohonen SOM	Chromatographic data	(Cabrita et al., 2012)

applied or not			
Classification tools for separating red wines according geographic origin and according variety	MLP 11-8-4	11 oenological descriptors	(Bednárová et al., 2013)
	MLP 12-6-3	12 oenological descriptors	
A classifier that discriminates subregion production of wines form UV-VIS-IR spectra	MLP	A set of specific wavelengths selected by PCA	(Martelo-Vidal and Vázquez, 2014a; 2014b)
Classification tools to segregate sines according region or subregion of origin, from metal content profiles	CPNN 14x14x19	19 element contents	(Šelih et al, 2014)
	CPNN 7x7x19	19 element contents	
Classification tools for wines according variety, vintage or winery of origin, based on antioxidant activity	PNN	6 antioxidant related indexes	(Hosu et al., 2014)
	PNN	6 antioxidant related indexes	
	PNN	6 antioxidant related indexes	

Table 3. Analytical methods and sensory devices

Approach	**Architecture**	**Inputs**	**Reference**
Electronic nose based on resistance sensors to recognize vintages	TDNN (Time Delay Neural Networks)	Sensor outputs and the last time sensor outputs	(Yamazaki and Ludemir, 2002; Ludemir and Yamazaki, 2003)
Electronic nose based on resistance sensors to recognize adulteration in wines, made by additions of methanol, ethanol or other wines	Mixture-of-experts	Sensor outputs	(Penza and Cassano, 2004a)
Electronic nose based on resistance to correspond sensor inputs with chemical composition	MLP	Resistive multisensor array signal	(Penza and Cassano, 2004b)
Electronic tongue based on impedance sensor to recognize wines of several kinds	Several MLP	Sensor outputs	(Riul Jr. et al., 2004)
Taster based on Headspace-SPME-GCMS for wine classification	MLP	Aroma compositions of wines	(Tiefenbrunner et al., 2009)
Electronic tongue based on amperometric sensors for polyphenol content determination	MLP 84-10-2	Voltammograms	(Cetó et al., 2012a)

Bioelectronic tongue based on enzymatic sensors for polyphenol content determination	MLP 128-6-2	Voltammograms	(Cetó et al., 2012b)
Bioelectronic tongue based on enzymatic sensors for polyphenol content identification	MLP 3-7-11	PCA data of voltammograms	
Electronic nose based on resistance sensors to classify different types of wines	MLP and PNN (Probabilistic neural networks)	Sensor outputs	(Aguilera et al., 2012)
Electronic nose for wine classification with neural network acting as an associative memory	Chaotic neural network	Up to 13 compound concentrations	(Fu et al., 2012)
Low-cost, DIY electronic nose based on resistance sensors for classification of samples	MLP	Sensor outputs	(Macías et al., 2013)
Electronic tongue based on voltammetric sensors for chemical analysis that classify cava wines according to dryness	MLP 96-4-2	Voltammograms	(Cetó et al., 2014)
Software applications based on spectrophotometric measurements tor	MLP 4-4-1	Antioxidant related	(Hosu et al., 2014)

predict antioxidant activity of wines		indexes	
Electronic tongue based on to predict an expert panel score of a wine	MLP 80-6-1	Voltammograms	(Cetó et al., 2015)
Applications to determine several chemical concentrations in a wine from spectral data	MLP	Absorbance peaks in UV-VIS-NIR	(Martelo and Vázquez, 2015)
Electronic nose for real time monitoring of the evolution of a wine	PNN	Sensor outputs	(Lozano et al., 2015)

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Table 4. Decision making and production issues

Approach	Architecture	Inputs	Reference
Optimization of critical processing parameters for specific results	MLP	Must composition and processing choices	(Vlassides et al., 2001)
Optimization of a blending system to produce wines with specific aroma	Backpropagation network	Three fractional compositions of blends	(Ferrier and Block, 2001)
A database with manager system to assist blending in wine production	Backpropagation network	Physical and chemical profiles of samples	(Ren and Ii, 2006)
An early prediction system for failed fermentations	MLP	Total sugar, density and alcoholic degree	(Román et al., 2011)
An early prediction system for failed fermentations	MLP	Total sugar, alcoholic degree and density	(Urtubia et al., 2012)
An RFID system for quality tracking and quality evaluation in	Perceptron	Quality tracking records	(Wang et al., 2012)

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wineries			
FTIR-based predictive method for quality assurance of wines	MLP	IR Spectra data, variety, year, barrel type	(Agatonovic-Kustrin et al., 2013)
Predictive models for tartaric acid precipitation to optimize wine production	MLP	Fourier transform Infrared spectroscopy data	(Malacarne et al., 2013)
Optimization of the valorization process of lees as winery by-products	MLP	4 experimental factors of ultrasound assisted extraction	(Tao et al., 2014)

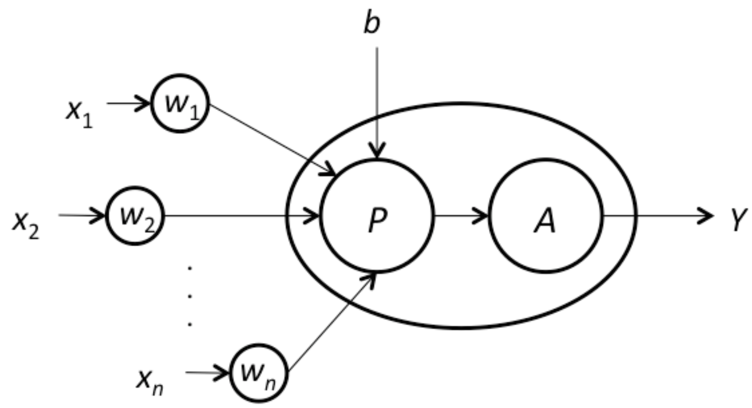


Figure 1. Scheme of an artificial neuron. Inputs *x*, coming from other neurons or not, balanced by its weights *w* are collected and summed according a bias *b* by means of the propagation rule *P*. Activation function *A* establishes then activation status. Output signal is produced by the output function *Y*, which is a lineal combination of input values.

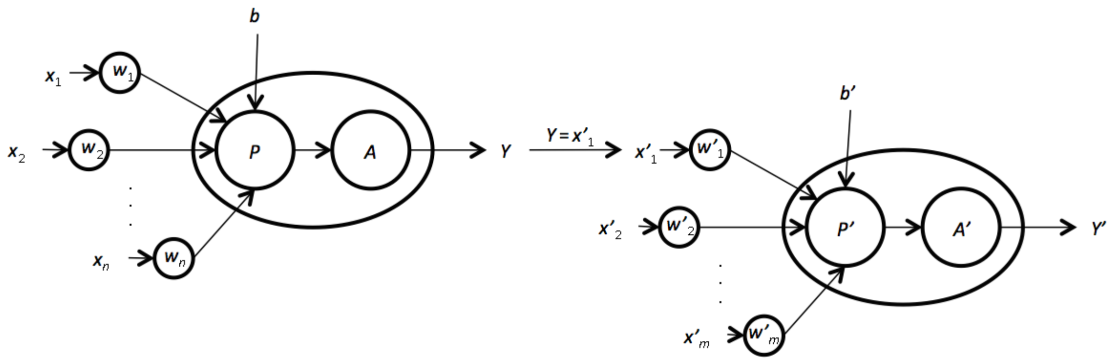
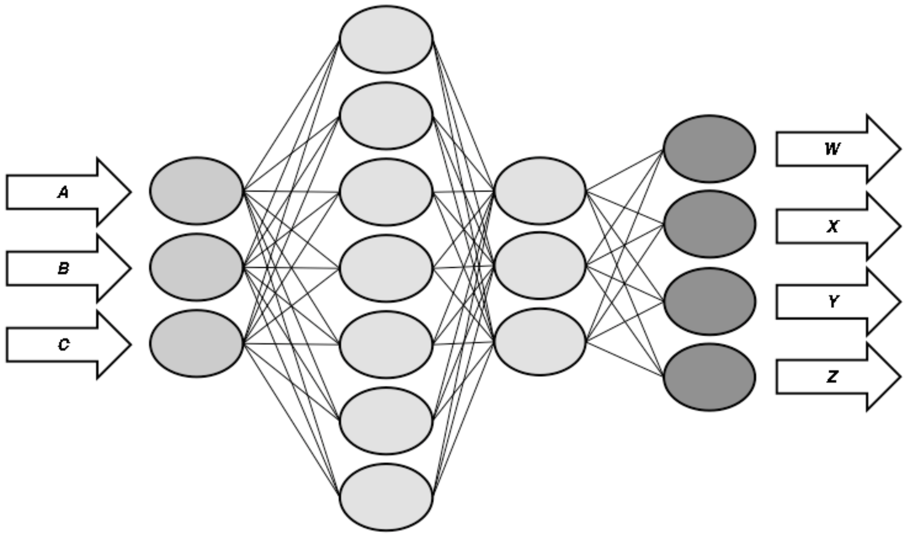


Figure 2. Synaptic connection between neurons of different layers.

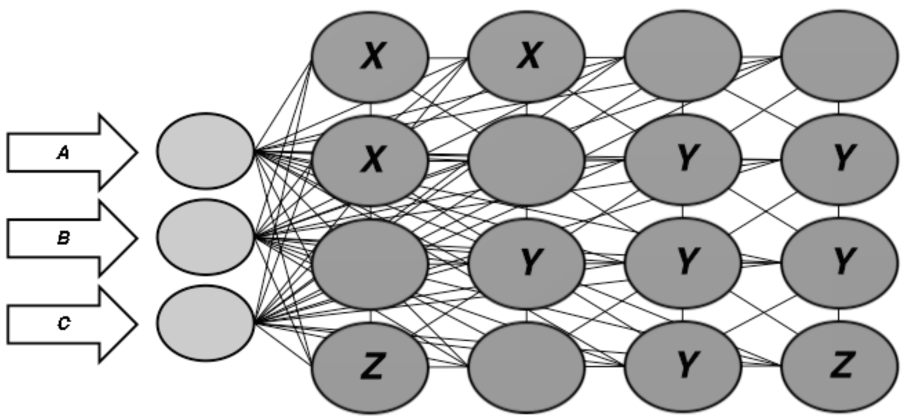
Neural networks architectures

- **Supervised Learning**
  - Perceptron
  - Multilayer Perceptron
  - Backpropagation
  - Adaline and Madaline
  - Time Delay Neural Network
  - Learning Vector Quantization
- **Unsupervised Learning**
  - Hopfield Networks
  - Kohonen Self-Organizing Maps
  - Neocognitron
- **Hybrid Learning**
  - Radial Basis Function
  - Counterpropagation
- **Reinforcement Learning**

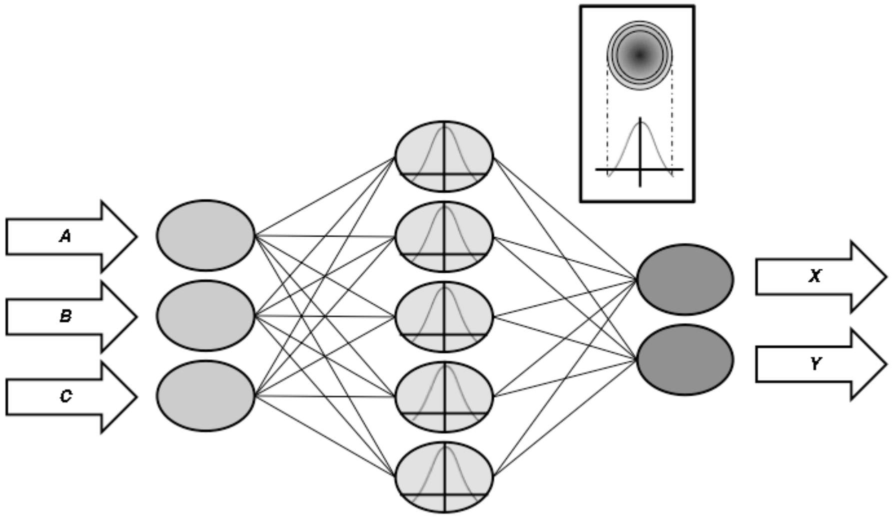
Figure 3. Typical artificial neural networks architectures according to learning type.



MLP



Kohonen SOM



RBF

Figure 4: Some of the most extended neural networks as they are commonly depicted. Medium grey nodes stand for input neurons; dark grey for output nodes; light grey for intermediate, hidden neurons. *A* to *B* represent input variables, while *W* to *Z* output variables or categories. In the Kohonen SOM the competitive layer, in dark grey, shows a feature map with three regions.

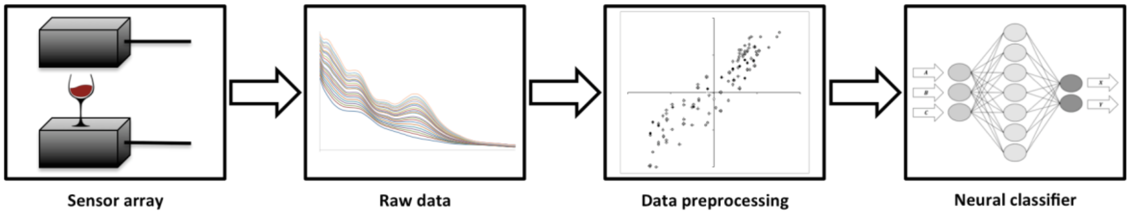


Figure 5. Scheme of a bionic sensory device based on artificial neural networks. Four stages are traversed by signal. First place, the sensor array retrieves analytical data form samples. Then, raw data is taken and commonly preprocessed to reduce its dimensionality and make it suitable for the classification stage.