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Combination of machine learning and intelligent sensors in real-time quality control of alcoholic beverages

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Abstract

Machine learning (ML) featured on its ability of learning and extracting features from a large set of data and automatically building statistical models. Through cooperation with intelligent sensors, which is designed to imitate human organs to analyze the sensory characteristics of foods, ML-based intelligent sensory systems such as electronic nose (E-nose) and electronic tongue (E-tongue) are developed for sensing applications in food industry. Consumption of alcohol beverages keep growing worldwide in recent years and fraudulent activities are stimulated due to the high price of alcoholic drinks, which motivates the application of intelligent sensory technology with high efficiency and accuracy for real-time quality control. Thus, this paper firstly summarizes the novel intelligent sensors that is suitable for sensory evaluation and the advanced ML algorithms used to create intelligent systems. Then the paper describes the mechanism of commercial ML-enabled intelligent devices and summarizes their practical sensing applications on the real-time quality control of a variety of alcoholic beverages, in term of detection of frauds and adulterations, aroma analysis, monitoring of the production process, and correlation with human sensory perception. Finally, the potential applications and future opportunities of ML-enabled intelligent sensor systems in the alcohol industry are discussed.

Keywords: machine learning; intelligent sensory; electronic nose; electronic tongue; alcoholic beverages; quality control.

Practical Application: ML-enabled intelligent sensory systems implement the real-time quality control of alcoholic beverages.

1 Introduction

Machine learning (ML) featured on its ability in learning and automatically extracting patterns and features from a given set of data that traditionally requires a domain expert to identify. In recent years, ML has been applied in collection, analysis, and interpretation of substantial sensory information, which replaces traditional sensing techniques with massive datasets and poorly understood models. In recent years, deep learning (DL) that imitate the structure and function of the human brain is developed to use artificial neural networks (NN) to perform complex scientific computations (Arsenovic et al., 2017). DL algorithms such as BP-NN, CNN, and PNN have shown outstanding advancement when dealing with a large set of samples with high accuracy and efficiency (Pan et al., 2014; Ha et al., 2020). ML has been widely used in dealing with complex sensory data in multiple food science fields such as wine, beer, milk, and apples (Farah et al., 2021; Hou et al., 2022; Zou et al., 2022).

Sensors that perform dedicated signal processing functions when it senses the appropriate input such as color, touch, and taste are called "intelligent sensors". The role of the signal processing includes reinforcement of inherent characteristics of the sensor device and enhancement of input signals for extracting the useful features of the food samples. For sensory evaluation purposes, the intelligent sensors are designed to imitate human organs to analyze the sensory characteristics of foods. Through cooperation with emerging ML algorithms, intelligent sensory systems such as electronic nose (E-nose) and electronic tongue (E-tongue) are created for sensing applications in food industry (Sanaeifar et al., 2017; Wang et al., 2020, 2022; Zhang et al., 2021; Kaur et al., 2022).

Consumption of alcoholic beverages keep growing each year worldwide. The value of alcohol ecommerce grows by 11% in 2019 across 10 core markets and is expected to increase by 42% in 2022, to reach US $24 billion (International Wine & Spirit Research, 2021). Quality control of alcoholic beverage heavily depends on the sensory evaluation of trained expert; however, human panels are usually expensive, subjective, and it is difficult to establish a corresponding mathematical model (Aleixandre et al., 2018). ML-enabled intelligent sensory systems provides a real-time quality control technique that is non-destructive, high-speed, good repeatability, reliable results, no sensory fatigue, and no complex sample preprocessing process (Watson et al., 2021).

This review firstly summarizes the novel intelligent sensors that is suitable for sensory evaluation and the advanced ML algorithms used to process complex sensory data. Then the

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paper introduced the commercial ML-enabled intelligent sensory systems (E-nose and E-tongue) for real-time quality control and summarizes their practical sensing applications on the authentication of a variety of alcoholic beverages, in term of detection of frauds and adulterations, aroma analysis, monitoring of the production process, and correlation with human sensory perception. Finally, the review discussed the challenges of current ML-enabled intelligent sensory systems and provided an outlook on the future opportunities.

The scientific literature was collected from Web of Science, Scopus, PubMed, Google Scholar, and Research Gate using keywords including "intelligent sensors", "machine learning", "alcoholic beverages", "electronic nose", "electronic tongue", "authentication" and so on. We have reviewed the most relevant progressive studies with an emphasis on the past 5 years. The search results were manually refined for relevance and evaluated to remove multiple and duplicate references.

2 Intelligent sensors for sensory detection

The intelligent sensors employed for sensory detection mainly including gas sensors, electrochemical sensors, biosensors, and optical mass sensors (Jiang et al., 2018). The intelligent sensors create reversible changes of electrical properties through reacting with analyses. Measurable electrical signals are then being used to do pattern recognition and classification. The measurement of electronic signals is typically obtained through measurement of the output voltage of the sensor and characterization of the output voltage pattern by parameters, response time, and recovery time (Kaur et al., 2022).

2.1 Metal oxide semiconductor (MOS) sensors

MOS is one of the most common sensing materials used in intelligent sensory evaluation. MOS are primarily metal-oxides or semi-conducting materials such as tin dioxides, zinc oxides, iron oxides, and titanium dioxide. MOS sensors are commonly used in E-nose for food aromas determination and discrimination because of its appropriateness for various gases (Wang et al. 2010). Based on the types of the sensing materials (reduction or oxidization), there are two types of gas sensors: 1) n-type sensors (made from oxides of zinc, tin or iron) which respond mainly to reducing compounds such as H_2S; 2) and p-type sensor (made from oxides of nickel oxides or cobalt oxides) which respond mainly to oxidizing compounds such as O_2 (Tan & Kerr, 2018a; Tan & Xu, 2020). The p-type sensors are most frequently used sensors in E-nose due to high sensitivity as well as high selectivity (Nazemi et al., 2019). The working principle of MOS sensors is described in Figure 1.

It was reported that MOS gas sensors can detect various food volatiles such as alcohols, organic acids, esters, aldehyde and ketones (Tan & Kerr, 2018b). The detection threshold of commercial MOS sensors is normally between 1 ppm–1000 ppm. Even though the MOS sensors are sensitive and selective, they need to operate at high temperatures between 150 and 400 °C that require a significant amount of energy and need a relatively long time for heating before they are ready to take measurements (Nazemi et al., 2019).

2.2 Conducting polymers (CP) sensors

Conducting polymers (CP) is also called intrinsically conducting polymer (ICP), which comprise of conducting particles such as polypyrrole, polyaniline, and polythiophene, interspersed in an insulating polymer matrix (Megha et al., 2018; Tan & Xu, 2020). The working principle of CP is through the reaction between sensing materials and volatiles, which introduces impunity into the sensing materials (Figure 2). Then the doping level in CPs induces a transfer of electrons to or from the analytes and results in a change in conductivity (Bai & Shi, 2007).

CP gas sensors might be the second commonly used gas sensor after MOS sensors, which shows high sensitives (≥ 10 ppm) to many food-derived volatiles such as aldehyde, acetates, and alcohols (Tan & Xu, 2020). Compared to MOS sensors, CP sensors have good mechanical properties (more durable) and do not require extra heating for operation which save a considerable cost for analysis. In addition, conducting polymers in CP sensors are easily to be synthesized through chemical or electrochemical processes and the structure of CP molecular chains can be modified by copolymerization or structural derivations (Megha et al., 2018). However, CP sensors

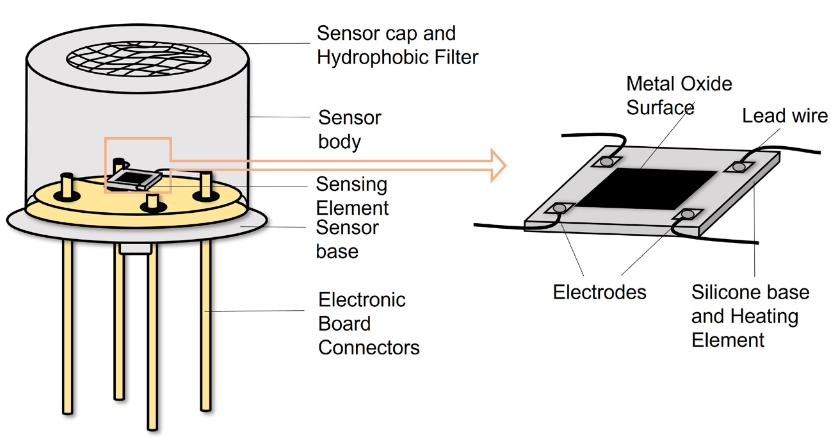

Figure 1. The working principle of metal oxide semiconductor (MOS) sensors.

are susceptible to humidity and still need relatively high operating temperatures (Megha et al., 2018).

2.3 Acoustic wave (AW) sensors

An acoustic wave (AW) sensor normally composes of a piezoelectric substrate coated with sensing material and two interdigital transducers (one input and one output) (Go et al., 2017). There are two types of acoustic wave gas sensors: 1) the acoustic wave propagates on the surface of the substrate is called surface acoustic wave transducers (SAW) sensor, and 2) the wave propagates through the substrate is called bulk acoustic wave transducers (BAW) sensor (Go et al., 2017). When the compatible analyte exposed to sensing material, the mass of gas-sensitive membrane of the sensor is changed and results in a change in SAW velocity and attenuation. SAW gas sensors coupling with Solid Phase Microextraction (SPME) has been used for the rapid detection of food pathogens and spoilages, including organic acids such as acetic acid, ethyl acetate, hexanal, and alcohol such as wine and beer products (Lamanna et al., 2020; Tan & Xu, 2020).

2.4 Potentiometric chemical (PC) sensors

Potentiometric chemical (PC) sensor measures the voltage difference between the working electrode and the reference electrode. Reference electrode is submerged in an electrolyte solution and keeps constant voltage during the measurement (Figure 3). Commonly used membranes for PC sensors include glass, crystalline/solid-state, liquid, and polymer materials (Moreno et al., 2018). PC sensors can be used for the determination of H^+, Na^+, Cl^-, F^-, Ca^{2+}, K^+, Ca^{2+}, Cl^- and NO^{3-} in solution phase (Ding et al., 2017). PC sensors are one of the most commonly used sensors for E-tongue. Since PC sensors can select specific or less specific membranes for its electrodes, they have been used for identification and classification of food components in a very broad range including various alcoholic beverages such as beers and wines (Nery & Kubota, 2016). PC sensors showed good accuracy, low cost, and rapid detection in food quality control (Kaur et al., 2022). However, PC sensors are sensitive to temperature. Furthermore, the membrane of the PC sensors may adsorb the solution components, which can affect the nature of the charge transfer (Ciosek & Wróblewski, 2011).

2.5 Biosensors

Biosensors are electronic sensors employing biomaterials as their sensing medium such as enzymes, receptors, and antibodies (Fuentes et al., 2021). The working principle of biosensors typically introduced by the interaction of a biological element with the sample as a result of a series of biochemical reactions, such as enzyme-substrate reaction that initiate the transport of electrons, which is further transcribed into electrical signals as shown in Figure 4 (Tan & Xu, 2020). Biosensors are widely used in food industries and the commercial biosensors including voltammetric sensors, impedimetric sensors, potentiometric sensors, and conductometric sensors have been applied in E-tongue instrument for the detection of alcohols, phenols, acids, and water-soluble vitamins in food products (Fuentes et al., 2021).

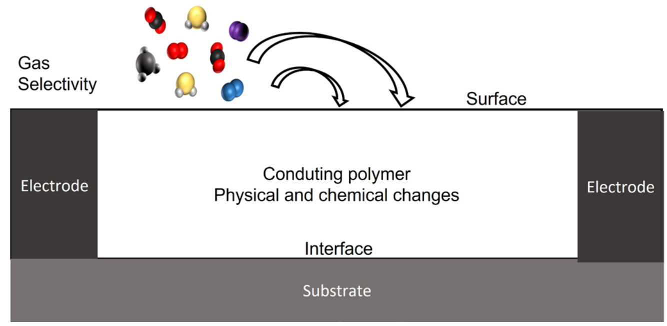

Figure 2. The working principle of conducting polymers (CP) sensors.

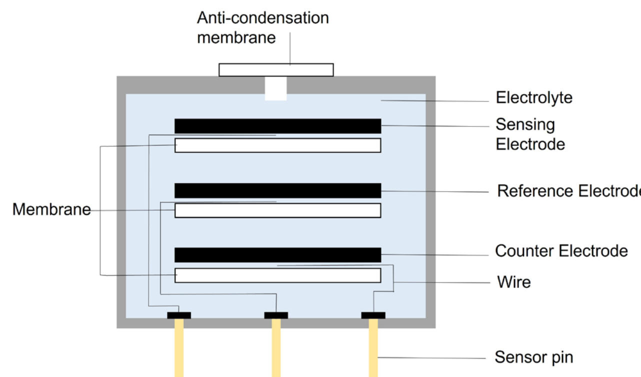

Figure 3. The working principle of potentiometric chemical (PC) sensors.

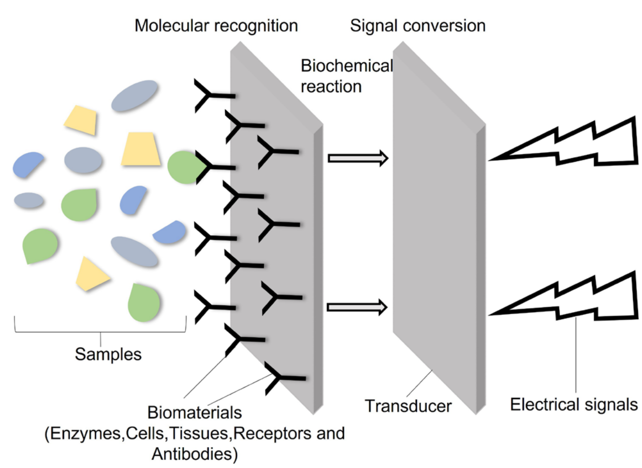

Figure 4. The working principle of voltammetric chemical (VC) sensors.

The biosensors play an important role in the detection of food compositions with ultra-low concentration in a very sensitive, accurate, and selective way (Mahato et al., 2018).

3 Machine learning algorithms

Machine learning (ML) builds mathematical model by training with high quality datasets before being implemented into the intelligent sensory system (Figure 5). Pattern recognition is an

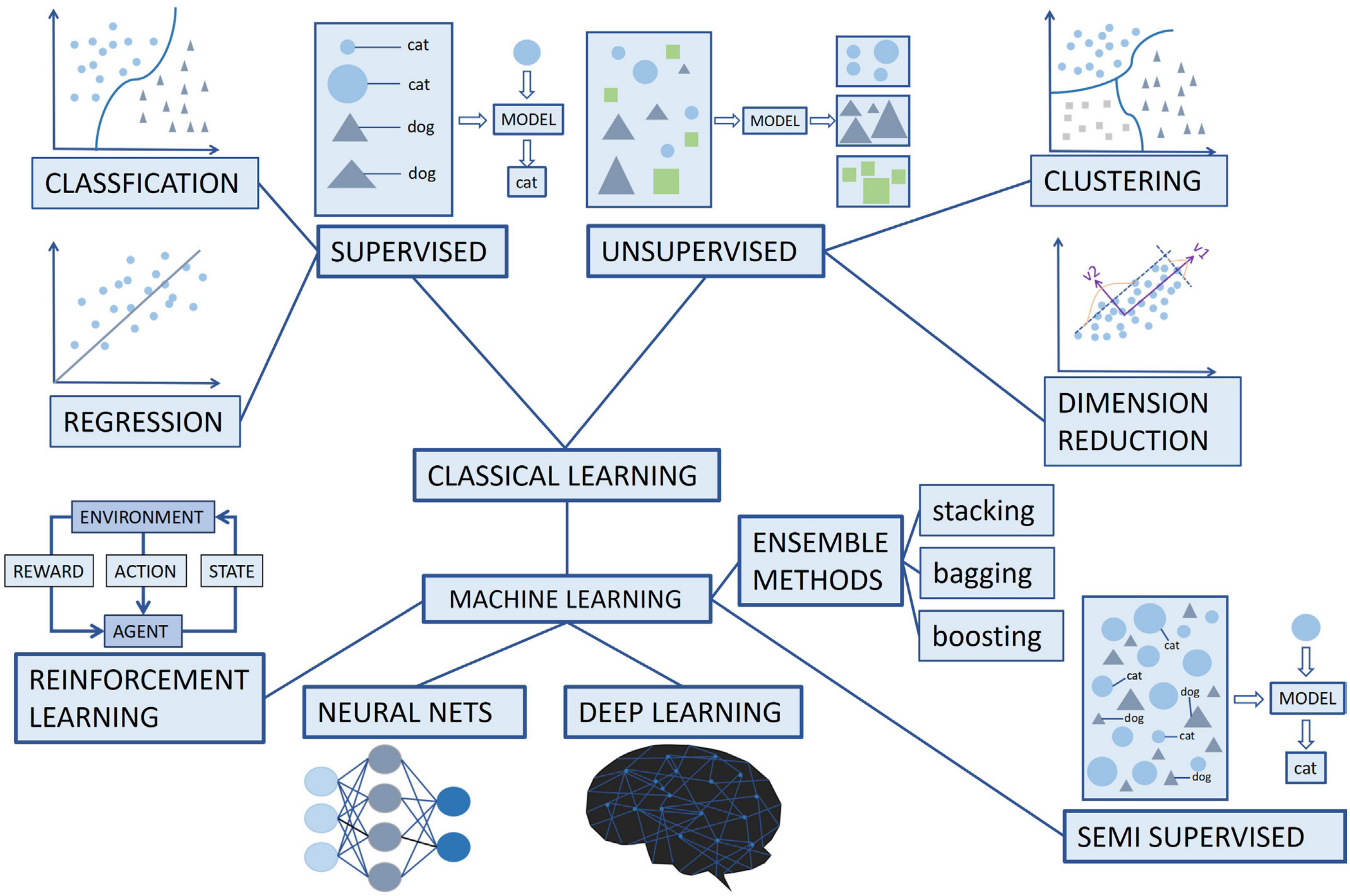

Figure 5. Schematic diagram of mechanism of ML algorithms.

effective data mining technique that applies various mathematical models to process the signals collected by intelligent sensors and yield characteristic sensory information in order to rapidly discriminate or classify the food samples (Khan et al., 2019). NN algorithms (such as BP-NN, CNN, and PNN) are highly efficient in terms of feature learning and extraction, which require less manual input when compared to non-NN ML algorithms such as linear regression, PCA, SVM, and RF (Ha et al., 2020).

3.1 Partial least squares discriminant analysis (PLS-DA)

PLS-DA is a popular machine learning tool that is attracting increasing attention as a useful feature selection and classification. PLS-DA illustrates the relationship between the independent variable X (response signal matrix of sensors) and the dependent variable Y (corresponding to the actual physical quantity), and established a standard curve to predict the value of the unknown point (Brereton & Lloyd, 2014). PLS-DA might be considered as a "supervised" version of PCA since it reduces the dimensionality but with full awareness of the class labels at the same time (Botella et al., 2009). However, it is important to note that its role in discriminant analysis can be easily misused and misinterpreted, because it is prone to be overfitting and the cross-validation is critical when using PLS-DA as a feature selector, classifier or even just for visualization (Brereton & Lloyd, 2014).

3.2 Soft independent modeling of class analogy (SIMCA)

SIMCA is a pattern recognition method based on PCA, which is a classification analysis method (Wold, 1976). Firstly, SIMCA performs a PCA on each of the predefined classes from the training set. PCA was performed using a full cross-validation; PCA models retain a certain number of significant principal components and the outliers were eliminated. Secondly, SIMCA obtains a basic impression of sample classification and establishes corresponding class models for each type of sample, and then use these class models to perform discriminant analysis to define the category of unknown samples. A sample can be assigned to several classes if they overlap or are very close to each other. If the sample belongs to none of the classes, it is possible to be considered as a "rejection class" (Hu et al., 2016). The advantage of SIMCA over other discrimination analysis is that it is very easy to add new classes. This method works very well for authenticating products with very different X values.

3.3 Back propagation artificial neural network (BP-ANN)

As a common ANN model in machine learning, BPANN is a promising tool for solving complex nonlinear modelling problems (Pham et al., 2017). BPANN uses a nonlinear differentiable function to train a multilayer network, which is divided into input layer, hidden layer, and output layer. BPANN is able to declare the nonlinear relationships within the sample data without assuming a specific relationship between the input and output in advance. The model has good prediction accuracy, strong anti-interference ability, and strong classification and prediction ability. The advantage of BPANN includes: 1) simple structures and easy operation, 2) sophisticated nonlinear mapping from input to output, and 3) self-study ability for further improvement and development (Fang & Jiménez-Guerrero, 2021).

3.4 Support vector machine (SVM)

SVM is a type of machine learning algorithm that can be used for classification, regression and outlier's detection. Since its inception, SVM is efficient at various tasks and has shown excellent characteristics in solving complex problems such as nonlinearity, high-dimensional space, small samples and local poles. SVM has been widely used in function approximation, pattern recognition, signal prediction, and fault diagnosis. SVM is also effective in high dimensional spaces and in cases where number of dimensions is greater than the number of samples. Because of its flexibility, high performance, and compute efficiency, SVMs have become a mainstay of machine learning (Raghavendr & Deka, 2014).

3.5 Probabilistic neural network (PNN)

Probabilistic neural network (PNN) is a non-parametric artificial neural network that can estimate the probability density function of a given set of data (Mohebali et al., 2020). PNN is a feedforward neural network developed from radial basis network and is suitable to solve classification and pattern recognition problems. The hierarchical model of PNN consists of an input layer, a pattern layer, a summation layer, and an output layer. The input layer transfers the input signals to each node of the mode layer. Then the mode layer performs a weighted summation of the input vectors passed by the input nodes, then passes it to the summation layer after a nonlinear operation. The output layer selects the state mode that is the largest output of the summation layer as the classification result. PNNs is a promising tool in solving scientific and engineering challenges such as labeled stationary data pattern classification, data pattern classification in which the data has a time-varying probabilistic density function, and so on (Mohebali et al., 2020).

4 ML-enabled intelligent sensory systems

4.1 Electronic nose (E-nose)

E-nose is mainly composed of three parts: a set of sensors, signal processing system and pattern recognition system. The sensor part adopts a plurality of gas-sensitive sensor arrays with different selectivity, and uses its cross-sensitivity to various gases to convert the effects of different molecules on its surface (Kaur et al., 2022). It can form a measurable physical signal group that can be easily calculated, classified, and identified. Many different technologies of sensors and biosensors have been implemented so far (Kimmel, et al., 2012). Another superior feature of E-nose over other devices is its employment of chemometric data analysis that reduces the time of analysis. Various patter recognition models can be used for E-noses data post-processing, including multiple machine learning models that keep developing in this field (Sanaeifar et al., 2017). The selection of a pattern analysis model depends on the type of data acquired as well as the purpose of the analysis (Figure 6).

4.2 Electronic tongue (E-tongue)

E-tongue instrument has a variety of transduction principles (mass, optical, or electrochemical) and the electrochemical sensors (potentiometric, amperometric, voltammetric, or impedimetric sensors) are the most widely used design (Kimmel et al., 2012). The work principle of E-tongue is to imitate human taste system: a sample preprocessor is firstly to convert the features of liquid sample into electronic signals like the taste receptor in the oral cavity (Figure 6). Then the sensors/biosensors array captures the signals and transmits it to the data processing system, which works as the neural sensory system in human brain. Finally, the data processing and pattern recognition system in E-tongue analyze the data using multivariate pattern recognition models (Lvova et al., 2015; Śliwińska et al., 2014).

5 Application of ML-enabled sensory systems for real-time quality control of alcoholic beverages

5.1 Detection of frauds and adulterations

The economic value of alcoholic beverage is highly associated with the brands, geographical origins, and years of aging

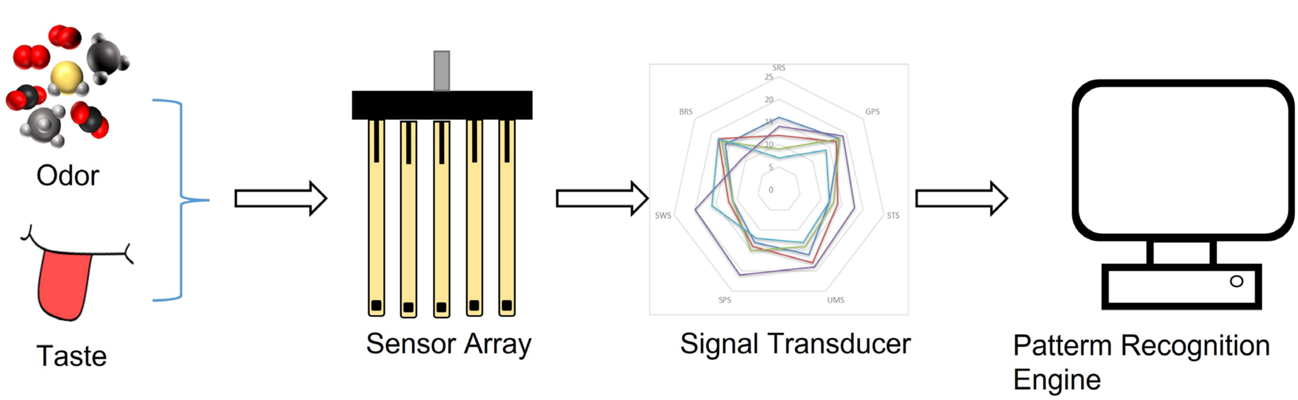

Figure 6. The schematic diagram of working principles of E-nose and E-tongue.

(Geană et al., 2020; Cao et al., 2021). In order to sell a higher price, some alcohol producers adulterate the information of their products, which damages the reputation of alcohol industry and the benefit of consumers (Zhang et al., 2019; Geană et al., 2020). ML-enabled sensory systems such as E-nose and E-tongue have been developed to establish a real-time quality control for alcoholic beverages (Geană et al., 2020).

A portable E-tongue system coupled with nonlinear BPANN recognition model successfully classified Chinese rice wine of 3, 5, 8 and 10 years of aging (Ouyang et al., 2013). The E-tongue consisted of three working electrodes (glassy carbon, gold and platinum) in a standard three-electrode configuration, using cyclic voltammetry technique to record signals. E-tongue coupled with discriminant analysis was used to identify the Chinese rice wine aged for 1, 3, and 5 years (Yu et al., 2017). Amino acid profiles were analyzed for the validation of the rice wine age and the correlation between the E-tongue responses and the amino acids was established by partial least squares regression (PLSR). In another study, the correlations between the E-tongue response and the sensory attributes were established via partial least square discriminant analysis (PLSDA) for identification of Chinese rice wine aged for 5, 7, 10, and 12 years (Yu et al., 2015). Furthermore, the PLSDA model for the taste-active compounds and the sensory tests showed that proline, fucose, arabinose, lactic acid, glutamic acid, arginine, isoleucine, valine, threonine, and lysine had an influence on the taste characteristic of Chinese rice wine (Yu et al., 2015).

Fusion of an E-nose and a voltammetric E-tongue system coupled with extreme learning machine (ELM) have been used as a rapid identification of red wines that differ in brands and grape varieties (Han et al., 2020). The fusion models derived from ELM were built with PCA scores, which showed superior performance (100% recognition rate) than individual intelligent technology. In case of distilled spirit, E-nose based on ultra-fast gas chromatography (fast GC E-nose) was used to discriminate a set of 24 raw spirits, 33 vodkas, and 8 whisky samples (Wiśniewska et al., 2016). DFA and SIMCA data analysis were used for discrimination of vodka, whisky, and spirits samples, and PCA was used to observe the variation among different types of liquors (Wiśniewska et al., 2016). Yang et al (2020) used E-nose coupled with back-propagation neural network (BPNN) technique to discriminate different brands of Chinese Fen liquors. A BPNN-based transfer-learning framework was trained on the liquor sample dataset, which presented a 93.4% accuracy in discrimination of the Chinese liquors.

5.2 Aroma analysis

Alcoholic beverages are favored due to the unique flavor characteristics. To identify the flavor composition of alcoholic beverage and tracing their changes during production process and storage, are hotspots in the alcohol industry. Combination of a mass spectrometry-based E-nose and E-tongue has been successfully used for evaluation of the flavor patterns of 13 commercial Korean distilled spirits (Kim et al., 2016). The flavor patterns of the distilled spirits were clearly identified through DFA analysis, which showed that the flavor pattern of the distilled spirits aged in oak barrels was not significantly different from that of the traditional distilled spirits (Kim et al., 2016).

In order to characterize the olfactory information of beers, E-nose coupled with Support Vector Machine (SVM) was developed for rapid detection. Twenty time-domain features and twenty frequency-domain features of E-nose sensors data were firstly extracted to represent the olfactory characteristics of beer (Men et al., 2018). According to variable importance in projection (VIP) scores, the forty subsets of multi-features with the best VIP score were established. Finally, the classification models were constructed based on SVM and the best parameter of SVM models were determined by Genetic Algorithm (GA). As a result, the developed GA-SVM model presented good classification performance in calibration set (81.67%) and testing set (96.67%), and the efficiency value was also the highest compared to other sets.

E-nose coupled with PCA, DFA, and soft independent modelling of class analogies (SIMCA) has been successfully used for the discrimination of characteristic aromas of four different alcoholic beverages including bourbon, brandy, cognac, and fruit spirits made from lemon (Surmová et al., 2020). SIMCA method successfully distinguished the point belonging to all groups without any approximation of graph fragments. Deep feature mining method for E-nose based on the convolutional neural network (CNN) combined with a support vector machine (SVM) to identify beer olfactory information (Shi et al., 2019). SVM replaced the full connection layer of the CNN to increase the generalization ability of the model, and the improved CNN-SVM model achieved deep feature automatic extraction of beer olfactory information which showed a good classification performance of 96.67%.

5.3 Monitor of the production process

Fermentation is a critical process that generally takes several days or even several months, which determines the ethanol content and affects the flavor of the final products. The E-nose and E-tongue are currently developed as a real-time quality control for detection of faults during fermentation in an economic and user-friendly manner (Sanaeifar et al., 2017).

E-tongue system was used to monitor the variation of alcohol contents in beers during fermentation. E-nose based on 13 gas sensors made with a metal oxide semiconductor (MOS) was proved to be an effective tool to quickly and accurately identify the alcohol content in a high spectrum of beers presents in the market (Voss et al., 2019). A hybrid E-tongue system based on potentiometric and voltammetric sensors was applied for the quality control of wine fermentation and storage process (Kutyła-Olesiuk et al., 2018). The sensor array formed by miniaturized ion-selective electrodes and glassy carbon electrodes. The effectiveness of the proposed system was compared to the standard reference methods used for quality control of wine production. Through PLS and Partial Least Squares-Discriminant Analysis (PLS-DA), the developed hybrid system allowed a reliable and effective discrimination of the wine samples during production.

5.4 Correlation with human perception

E-noses and E-tongues were not always well correlated to the results of sensory evaluation of human panels due to the complex compositions of alcoholic beverages that yield synergistic effect. However, recent advancements and breakthroughs in intelligent sensors and machine learning models can establish good correlations with sensory scores or with specific odors or flavors, which may substitute human sensory organs in the near future. Cetó et al. (2015) used a voltammetric E-tongue for standardized wine tasting and the results was correlated with a wine tasting sensory panel. A voltammetric array of sensors based on metallic and bulk-modified graphite electrodes was used as the sensing part, while chemometric tools such as LDA and artificial neural networks (ANNs) were used as the qualitative and quantitative modelling tools. The method showed a precision of 92.9% for the qualitative application, and a correlation coefficient of 0.830 for the quantitation. Furthermore, E-tongue was applied in the prediction of the global scores of red wines assigned by a sensory panel (Cetó et al., 2017). Signal responses obtained from E-tongue were preprocessed by fast Fourier transform (FFT) for the compression and reduction of signal complexity, and then the coefficients were used as inputs to build the qualitative and quantitative models using either LDA or PLS analysis. As a result, the E-tongue could provide a prediction of red wine global scores (0-10) from a trained sensory panel with a normalized NRMSE of 0.11, which may serve as a potential tool for quality control of wine industry. In addition, Aleixandre et al. (2018) compared an E-nose and human panel in the quantification of wines formed by binary mixtures of four white grape varieties and two types of red wines at different percentages. Both techniques were able to quantify the mixtures tested, but E-nose was proven to be much faster, simpler, and more objective than the human panel with high accuracy in quantification.

6 Conclusion

This paper presents a comprehensive literature review addressing the practical application of ML-enabled intelligent sensory systems on authentication of alcoholic beverages. The cross-sensitivity of intelligent sensors and multiple ML algorithms enhanced the accuracy and efficiency of real-time quality control of alcoholic beverages. After an appropriate training, intelligent devices such as E-noses and E-tongues provide qualitative and quantitative information of the alcoholic beverages, which may assist alcohol industry to predict the organoleptic characteristics of the products as well as make decisions regarding fermentation, aging, packaging, transportation and shelf-life.

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