

Novel digital technologies to assess smoke taint in berries and wines due to bushfires

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Abstract. Due to climate change, the higher incidence and severity of bushfires is a significant challenge for wine producers worldwide as an increase in smoke contamination negatively affects the physicochemical components that contribute to the lower quality of fresh produce and final products (smoke taint in wines). This reduces prices and consumer acceptability, impacting the producers and manufacturers. Current methods available to winemakers for assessing contamination in berries and wine consist of costly laboratory analyses that require skilled personnel and are time-consuming, cost prohibitive, and destructive. Therefore, novel, rapid, cost-effective, and reliable methods using digital technologies such as the use of near-infrared (NIR) spectroscopy, electronic nose (e-nose), and machine learning (ML) have been developed by our research group. Several ML models have been developed for smoke taint detection and quantification in berries and wine from different varieties using NIR absorbance values or e-nose raw data as inputs to predict glycoconjugates, volatile phenols, volatile aromatic compounds, smoke-taint amelioration techniques efficacy, and sensory descriptors, all models with >97% accuracy. These methods and models may be integrated and automated as digital twins to assess smoke contamination in berries and smoke taint in wine from the vineyard for early decision-making.

1 Introduction

Climate change effects in viticulture have been manifesting evidently in several worldwide winegrowing regions, as foretold some 15 years ago within a national climate change effect report in Australia [1]. Increased ambient temperatures and variability of water availability may have a variety of impacts on management practices with subsequent impacts on yield and berry quality traits. Furthermore, climatic anomalies, such as frosts, heat waves, and associated bushfires, are increasing in number and severity and with a broader window of opportunity (from September to April in the southern hemisphere) [2].

Bushfires happening close by vineyards can produce smoke clouds affecting the physiology of grapevine canopies, such as stomatal conductance, transpiration, and photosynthesis, with various lingering effects depending on the cultivar [3]. However, more importantly, they can impact the quality traits of grapes close to harvest if smoke contamination happens close to veraison, known as smoke taint. Smoke-derived compounds can bind with sugars in berries, producing glycoconjugates released to the wine during fermentation. Levels of smoke taint can vary from acceptable to spoilage depending on the level of contamination of berries used for winemaking [4]. The effect of smoke contamination on the berry chemistry and smoke taint in wines is well understood in the laboratory. However, the development of detection systems that can be available to grape growers and winemakers to assess smoke taint at different stages of wine production is almost inexistent. Hence, grape growers and winemakers need to rely either on costly laboratory analysis by sending samples from sentinel plants within a vineyard or doing micro vinification to assess the level of smoke taint by non-objective sensory methods. Any latter techniques are

time-consuming, cost-prohibitive, and do not provide high-resolution information from the whole grape production.

This work presents the latest advances in implementing new and emerging digital technologies coupled with artificial intelligence (AI) and machine learning (ML) to detect smoke taint and assess grapes and wines.

2 Materials and methods

2.1 Study site, sample collection

The study was conducted at the vineyards located at the University of Adelaide Waite Campus, Urrbrae, South Australia, Australia (34° 58' S, 138° 38' E) in the 2018-2019 season [5-8]. As described by Summerson et al. [6, 7], a total of five treatments of Cabernet Sauvignon grapevines were prepared. Two of the treatments consisted of control samples (i) with and (ii) without a fine mist of water at canopy level, while three treatments were smoked using barley straw at different levels (iii) low-density smoke (1.5 kg straw), (iv) high-density smoke (5 kg straw), (v) high-density smoke with a fine mist of water (5 kg straw) during one hour at seven days post veraison using an individual tent per treatment.

2.2 Sample preparation and glycoconjugate analysis

A total of 5 kg of berry bunches were collected in triplicates per treatment to produce wine samples using micro-vinification techniques described by Summerson et al. [7]. Samples of must from berries one day after application of smoke treatment and at harvest, along with

the wine samples, were analyzed for glycoconjugates and volatile phenols using stable isotope dilution analysis (SIDA) and gas chromatography-mass spectroscopy, respectively, as described in previous publications [7, 9, 10].

2.3 Near-infrared spectroscopy and electronic nose

Samples of berries (36 per treatment; three measurements per replicate), must, and wine (triplicates and three measurements per replicate) were analyzed using a portable NIR MicroPHAZIR™ RX Analyzer (Thermo Fisher Scientific, Waltham, MA, USA), which measures the chemical fingerprinting within 1596–2396 nm [6, 7].

A low-cost and portable e-nose was used to assess volatile compounds in the wine samples in triplicates. This e-nose consists of an array of nine different gas sensors as described by Gonzalez Viejo et al. [11], and results were analyzed using a code written in Matlab® R2021a (Mathworks, Inc. Natick, MA, USA) to obtain ten mean values from the most stable part of the curve [12].

2.4 Machine learning modeling

Classification and regression ML models were developed using artificial neural networks (ANN) with a Matlab® R2021a code written by the Digital Agriculture, Food and Wine group from The University of Melbourne (DAFW-UoM) [6, 7, 10, 13]. This code can test 17 different ANN algorithms to assess the ML models with the highest accuracy and performance based on cross-entropy for classification and means squared error (MSE) for regression models.

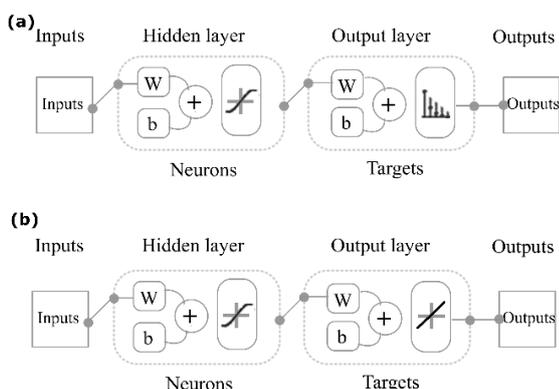


Figure 1. Artificial neural networks model diagrams for (a) classification and (b) regression showing the different layers of the models.

3 Results and Discussion

Table 1 summarizes the ML models developed to predict levels of smoke contamination and quality traits in wine and berries. Models were developed to predict the level of smoke contamination in grapevine leaves and berries using NIR measurements as inputs (accuracy: 98% and 97%, respectively) and in wine using e-nose outputs as

inputs (accuracy: 97%). Other models have been developed to predict glycoconjugates and volatile phenols in berries and wine, measuring wine samples for volatile compounds using the e-nose and chemical fingerprinting using the NIR, all with very high accuracy ($R > 0.98$). On the other hand, models to predict volatile compounds and intensity of different sensory descriptors related to consumers' acceptability and intensity of smoke aromas were constructed with outputs from the e-nose as inputs with very high accuracy ($R > 0.97$).

When deployed to assess new samples, all developed models presented high accuracy and maintained similar accuracies. Most research involving ML and AI does not present further deployments on new samples and is without basic statistical analysis to show that over or under-fitting was not present in the models. The latter makes it challenging to assess the real-world scenario applicability of these models in vineyards and wineries.

These ML models can also be used to implement smoke taint amelioration methods [2, 14, 15] to reduce the concentration of smoke-related compounds and the immediate effects on sensory attributes of wines produced. The latter could support the decision-making process for the winemaking of smoke-tainted grapes.

4 Conclusion

New and emerging digital technologies coupled with AI and ML have shown to be non-invasive and accurate for detecting smoke-related compounds in berries and predicting smoke taint in final wines. These technologies may enable grape growers and winemakers to measure smoke contamination in berries from the vineyards before harvest and predict smoke taint before the winemaking process. Results from the data acquisition and analysis can be in real-time, which would make possible effective decision-making in terms of differential harvesting. Furthermore, these techniques (NIR and e-nose) can also be implemented in the crushing, fermentation, and winemaking processes for smoke-related compounds and concentration so that winemakers can vary their time of fermentation in contact with skins and other procedures.

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Table 1. Summary of machine learning models developed to predict smoke contamination levels and quality traits in wine and berries.

Product	Type/ Algorithm	Inputs	Targets/Outputs	Accuracy	Publication
Grapevine leaves	Classification Levenberg–Marquardt	100 Near-infrared absorbance values (1596–2396 nm)	5 Levels and treatments of smoke taint	98%	[6]
Berries	Classification Levenberg–Marquardt	100 Near-infrared absorbance values (1596–2396 nm)	5 Levels and treatments of smoke taint	97%	[6]
Wine	Classification Levenberg–Marquardt	9 Electronic nose outputs in wine	5 Levels and treatments of smoke taint in wine	97%	[10]
Wine/Berries	Regression Levenberg–Marquardt	9 Electronic nose outputs in wine	20 Glycoconjugates and 10 volatile phenols in berries 1 h after smoking	$R = 0.98$	[10]
Wine/Berries	Regression Levenberg–Marquardt	9 Electronic nose outputs in wine	20 Glycoconjugates and 10 volatile phenols in berries at harvest	$R = 0.99$	[10]
Wine	Regression Levenberg–Marquardt	9 Electronic nose outputs in wine	17 Glycoconjugates and 7 volatile phenols in wine	$R = 0.99$	[10]
Wine/Berries	Regression Levenberg–Marquardt	100 Near-infrared absorbance values (1596–2396 nm) in berries	18 Glycoconjugates and 10 volatile phenols in berries 1 day after smoking	$R = 0.98$	[7]
Wine/Berries	Regression Levenberg–Marquardt	100 Near-infrared absorbance values (1596–2396 nm) in berries	18 Glycoconjugates and 10 volatile phenols in berries at harvest	$R = 0.98$	[7]
Wine/Berries	Regression Levenberg–Marquardt	100 Near-infrared absorbance values (1596–2396 nm) in berries	17 Glycoconjugates and 6 volatile phenols in wine	$R = 0.98$	[7]
Must and wine	Regression Levenberg–Marquardt	100 Near-infrared absorbance values (1596–2396 nm) in must	17 Glycoconjugates and 6 volatile phenols in wine	$R = 0.99$	[7]
Wine	Regression Levenberg–Marquardt	100 Near-infrared absorbance values (1596–2396 nm) in wine	17 Glycoconjugates and 6 volatile phenols in wine	$R = 0.99$	[7]
Wine	Regression Bayesian Regularization	9 Electronic nose outputs	Peak area of 8 volatile aromatic compounds	$R = 0.99$	[5]
Wine	Regression Levenberg–Marquardt	9 Electronic nose outputs in wine	Liking of 11 sensory attributes, emotion scale, and perceived quality plus the intensity of smoke aroma.	$R = 0.98$	[10]
Wine	Regression Bayesian Regularization	9 Electronic nose outputs	Smoke aroma intensity	$R = 0.97$	[5]