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Classification of Garlic Varieties with Fluorescent Spectroscopy Using Machine Learning

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Abstract: Machine learning techniques can produce fast, accurate and objective results in the analysis of agricultural products. These artificial intelligence-based systems are frequently encountered in studies on agriculture in the literature. This study reveals the usability of machine learning algorithms in classification of garlic cultivars using fluorescent spectroscopic data. For this, six types of garlic were used: Razgradski-11, Razgradski-12, Razgradski-115, Plovdivski-120, Yambolski-99 and Topolovgradski. In the first stage, the parsing analysis made from the fluorescent spectroscopic data of the garlics was carried out with seven different machine learning. The classification results of these seven types of machine learning algorithms were obtained. In the second stage, the classification results were obtained by adjusting the hyperparameters of each Machine Learning (ML) algorithm in order to control the improvability of the classification accuracy rates. Finally, performance metrics such as Specificity, precision, MCC, F1-Score of the classification processes obtained in the two stages were compared. In general, it was observed that the classification performances increased with the hyperparameter adjustment performed in the second stage. In this study, classification results with ML showed that fluorescent spectroscopy data of garlic strongly represented garlic species and provided high performance classification accuracy of 99.93% with Neural Network (NN), one of the machine learning methods using these data.

Keywords: Fluorescence Spectroscopic Data; Garlic; Hyper Parameter Tuning; Machine Learning Algorithms; Performance Metrics

1 INTRODUCTION

Garlic (Allium sativum L.) is a cereal product rich in minerals, vitamins, protein, polysaccharides, calcium, potassium and oligosaccharides. [1]. It is a potentially medicinal agricultural product with curative, therapeutic, antibacterial and antimicrobial properties in terms of medicinal properties of humans for hundreds of years [2, 3]. In many countries, garlic is recommended to be consumed by doctors because of these properties that it has in pain relief, calming, digestive and respiratory system disorders and cardiovascular disorders [4]. More than 200 phytochemical compounds contained in garlic and essential oils obtained from garlic contribute to the vitality and health of humans [5]. It has been suggested that garlic essential oil has many potentials such as antioxidant, antimicrobial [6, 7], antibacterial [8], antiviral [9] and biological activity [5]. Garlic has been used as a natural disinfectant in poultry, to sterilize hatching eggs [10]. Due to these benefits, its production continues to increase in the world, especially in countries such as China and India. The quality of garlic may vary according to the region, climate conditions, growing environment and variety where it is grown [11]. Growing conditions can affect the chemical composition of garlic, which will affect its bioactive compound content and quality [12]. Allicin content, antioxidant capacity and total phenolic contents may be different in garlic varieties [11]. Therefore, it is important to distinguish garlic varieties in terms of cultivation and use. Classification and separation process in fluorescent spectroscopy data using machine learning methods will eliminate the difficulties that experts working in this field will experience in classifying these data [13].

Fluorescence spectrometry has recently become a widely preferred method for dealing with the authenticity and quality of various foodstuffs due to its selective and high sensitivity as well as relatively low cost [14, 15]. Fluorescent spectroscopy and hyperspectral fluorescence imaging consider two unique fingerprints to examine compounds in foodstuffs [16]. Fluorescence spectroscopy can be used to determine the quality of plant and animal products [17]. Fluorescent spectroscopy can be used in dairy products, fruits, juices, oil, grain, etc. It is used to define, verify, classify the parameters needed in the processing, storage and storage of food products and to perform the optimization of these parameters in a non-invasive and fast way [18]. Studies using fluorescence spectrometry in the literature are examined below.

Botelho et al. (2017) suggested in their study that fluorescence spectroscopy can be used to distinguish four different coffee types grown in Minas Gerais State of Brazil [19].

Zekovic et al. (2012) used fluorescence spectroscopy for classification and analysis of cereal flours (rice, rye, corn, barley, wheat and buckwheat) to classify specified flour types by partial least squares separation analysis, principal component analysis and cluster analysis methods [20].

Karoui et al. (2007) performed fluorescence spectroscopy, principal component analysis (PCA) and factorial discriminant analysis (FDA) methods for the classification of samples of seven Swiss honey species according to their botanical origins [21].

Fang et al. (2021), in their study, proposed 4 different methods for the classification and characterization of pale lager beers grown by different manufacturers in China, using fluorescence spectroscopy data obtained in different ways. The best classification result was obtained with parallel factor analysis (PARAFAC) data fission and *k-nn* [22].

Liu et al. (2020) in their study, the accuracy of the verification and calibration sets with the partial least squares discriminant analysis (PLS-DA) algorithm was 86.96% and 92.54%, respectively, to demonstrate the usability of fluorescence spectroscopy to detect non-destructive, microbial and chemical spoilage indicators and freshness of beef. [23].

Bartolic et al. (2022) used two anti-invasive multispectral imaging (MSI) and optical fiber fluorescence spectroscopy methods to distinguish aflatoxin B1 (AFB1) from corn seeds from uncontaminated and contaminated seeds [24].

Sabanci et al. (2022) used fluorescence spectroscopy data and machine learning algorithms to classify red onion varieties in an objective and non-destructive way [13].

Ropelewska et al. (2022) used fluorescence spectroscopy data of three different tomato species to classify yeast-inoculated and non-inoculated tomato varieties by combining them with machine learning techniques [25].

Ropelewska et al. (2022), in their study, they classified the fluorescent spectroscopy data of five different onions grown in irrigated agriculture and onions grown in dry agriculture using machine learning methods [26].

As can be seen from recent studies, fluorescent spectroscopy data is used in the classification of liquid (oil, dairy products, and fruit juices) and food products. In this study, fluorescence spectroscopic data were used for the characterization and classification of garlic. Approaches to classify spectral data obtained from six different garlics using machine learning techniques add innovation to our study. In order for the proposed models to produce optimum results, the success of the methods has increased in general by performing hyper parameter analysis and performance metrics have been compared. Garlic producers can use recommended methods for processors to identify garlic species. This will be useful to ensure the purity of the species and to prevent mixing. The combination of machine learning and Fluorescent spectroscopy is a unique approach for objective, non-destructive and rapid differentiation of garlic species.

2 MATERIALS AND METHODS

This section presents the methods for analyzing and classifying six different garlic varieties. The block diagram of the proposed method in our study is given in figure1. First, fluorescent spectroscopy data of garlic cultivars were obtained. Then, the data set obtained from the received data was classified by Machine Learning algorithms. In order to increase the classification accuracy, the hyperparameters of the Machine Learning methods were adjusted and reclassified. Finally, the classification performances of the models were compared. All processes are explained in detail below. The block diagram of the study is given in Fig. 1.

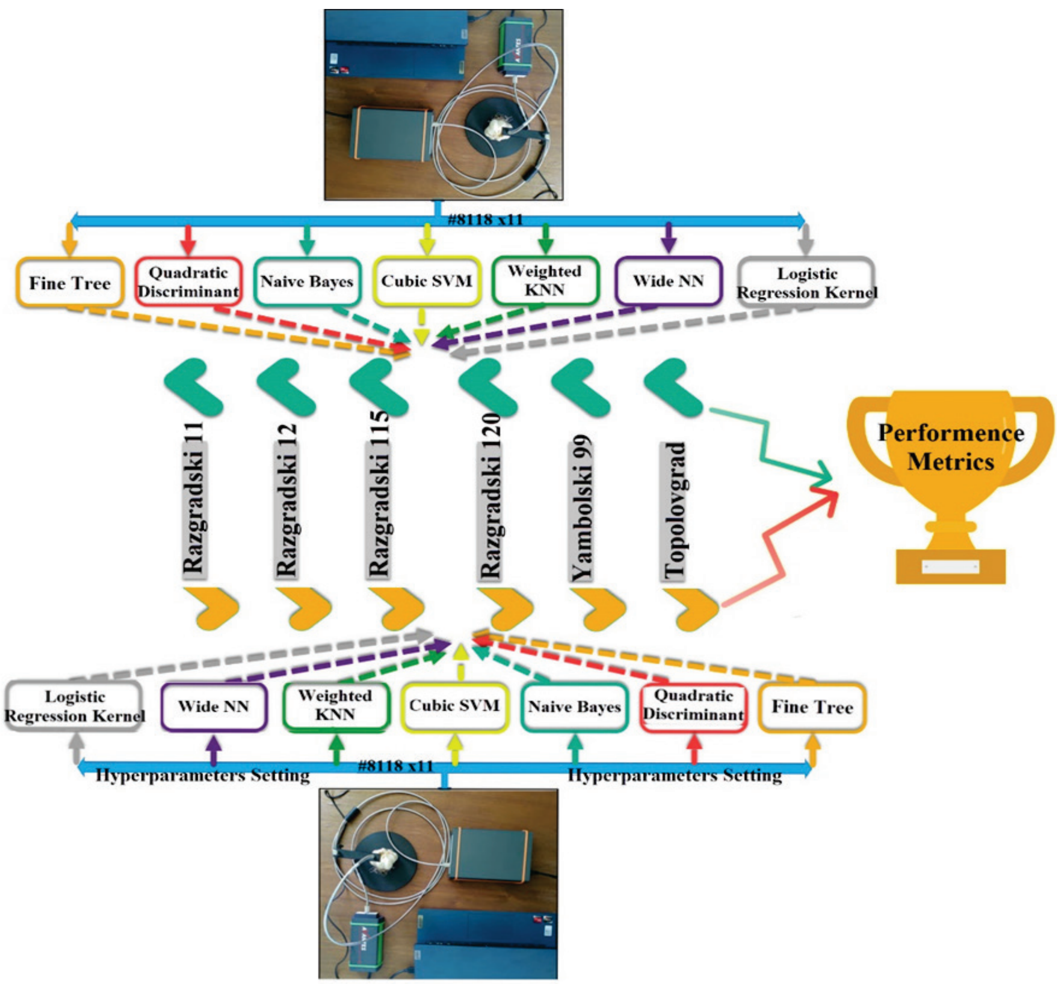

Figure 1 Block diagram of the study, obtaining data, classification with standard parameter values and machine learning methods, parameter optimisation and classification with machine learning methods, comparison of performances.

2.1 Dataset

The garlic used in this study consists of proprietary and breeding garlics. Six types of garlic and their main characteristics are given below.

Razgradski 11: Specimen of winter garlic characterized by medium-sized bulbs with closely spaced clippings. The bulb weighs 40 g. Dry matter content measured refractometrically 33%

Razgradski 12: Specimen of winter garlic characterized by medium to large bulbs with loosely arranged cloves. The bulb weighs 60 g. Dry matter content measured refractometrically 31%.

Razgradski 115: Specimen of winter garlic characterized by small bulbs weighing 30 g, cloves closely spaced. Dry matter content measured refractometrically 32%.

Plovdiv 120: Specimen of winter garlic characterized by medium-sized bulbs weighing 45 g, with densely arranged cloves. Dry matter content measured refractometrically 32%.

Yambolski 99: Specimen of winter garlic characterized by large bulbs weighing 70 g with densely spaced cloves. Dry matter content measured refractometrically 40%.

Topolovgrad: Specimen of winter garlic characterized by large bulbs weighing 70 g, with densely spaced cloves. Dry matter content measured refractometrically 30%.

The accessions that are the subject of the study are Razgradski 11, Razgradski 12, Razgradski 115, Plovdivski 120, Yambolski 99 and Topolovgradski were grown at the Maritsa" Vegetable Crops Research Institute in the period 2021-2022, with an experimental plot area of 4.8 m^2, according to the scheme 85 + 25 + 25 + 25×6 cm, according to the accepted technology for growing ripe garlic. Garlic was planted in mid-October and harvested in mid-June, after which it was left to dry in a storage room. The agro-technical events were carried out in the optimal terms for the culture.

2.2 Fluorescence Spectroscopy

Fluorescence is the light emission that remains after the absorption of ultraviolet light of a fluorescent component called a fluorophore, which absorbs energy of a certain wavelength and releases energy at a higher wavelength [17]. The Jablonski diagram showing the general principles of fluorescence spectroscopy is given in Fig. 2 and you can find detailed information in the related study [17].

The fluorescence study was carried out using a fiber-optic portable spectrometer model AvaSpec-ULS2048CL-EVO. The sensitivity of the spectrometer is in the range of 200 nm to 1200 nm. Its resolution is $\Delta\lambda = 5$ nm. An AvaLight High Power LED with an emission wavelength of 285 nm was used as an excitation source. The sources are of high power and generate a pulse spectrum signal at the output of the circuit. The signal from the source is taken to the bulbs by means of a U-shaped optical fiber. The useful fluorescence signal is measured in a direction that is less than 180° to the excitation radiation with the selected sample for analysis positioned vertically on a duralumin stand with a pitch black coating. The coating prevents glare and reduces aberrations. As shown in Fig. 3, a higher quality fluorescent signal is produced.

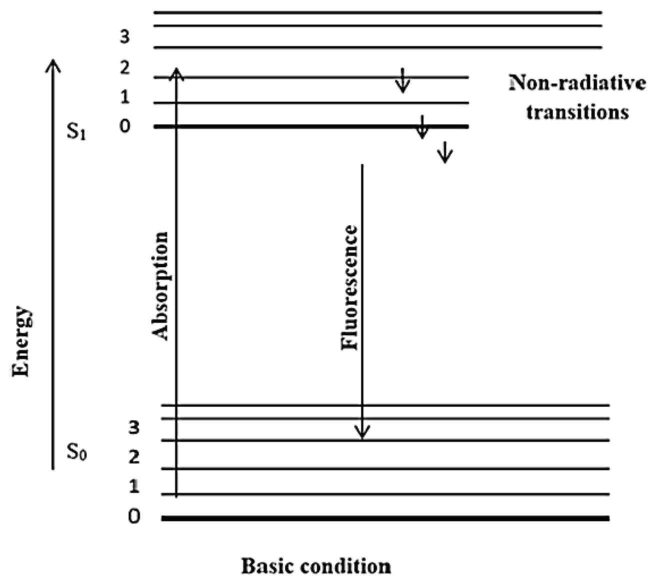

Figure 2 Representation of the basic principle of fluorescence spectroscopy with the Jablonski diagram

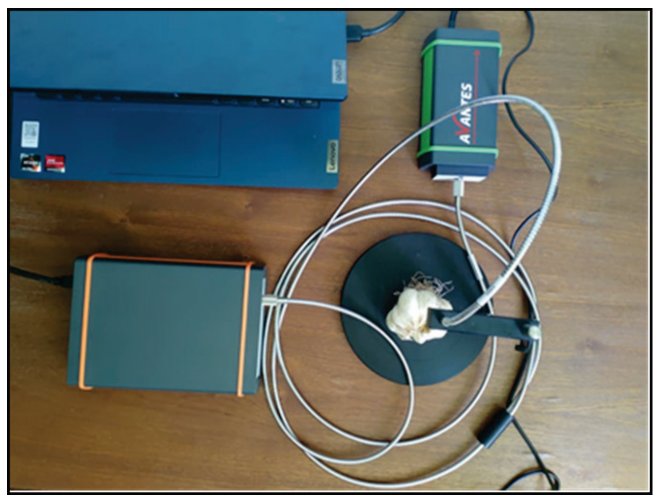

Figure 3 Fluorescent spectroscopy experimental setup

The fiber-optic installation makes it possible to record both the emission spectrum and the spectrum of the excitation source. The emission spectrum is defined by the emission wavelength distribution measured for one constant excitation wavelength, and the excitation by the dependence of the emission intensity measured for one scanning wavelength against the excitation wavelength. The spectral distributions are generated by means of two-dimensional graphs, as the abscissa shows the emission wavelengths for a specific bulb from a selected branch of garlic, and the ordinate shows the signal intensity. The signal is taken to the sample by means of prisms with a reflection coating with a reflection rate of 95 %. The signal from the bulb is captured by a system of lenses to compensate for chromatic aberration. The anti-reflective coating of the prisms, in turn, reduces the reflection coefficient to 0.2%. By means of an optical fiber with a core diameter of 200 µm with a step index of refraction and a numerical aperture of 0.22, the signal is taken to the detector. In the spectrometer, the light signal is converted to electrical-digital using a USB 2.0 wire, downloaded to a computer with AvaSoft8 software and exported to Excel. This allows analysis, processing and visualization of the results of the conducted research.

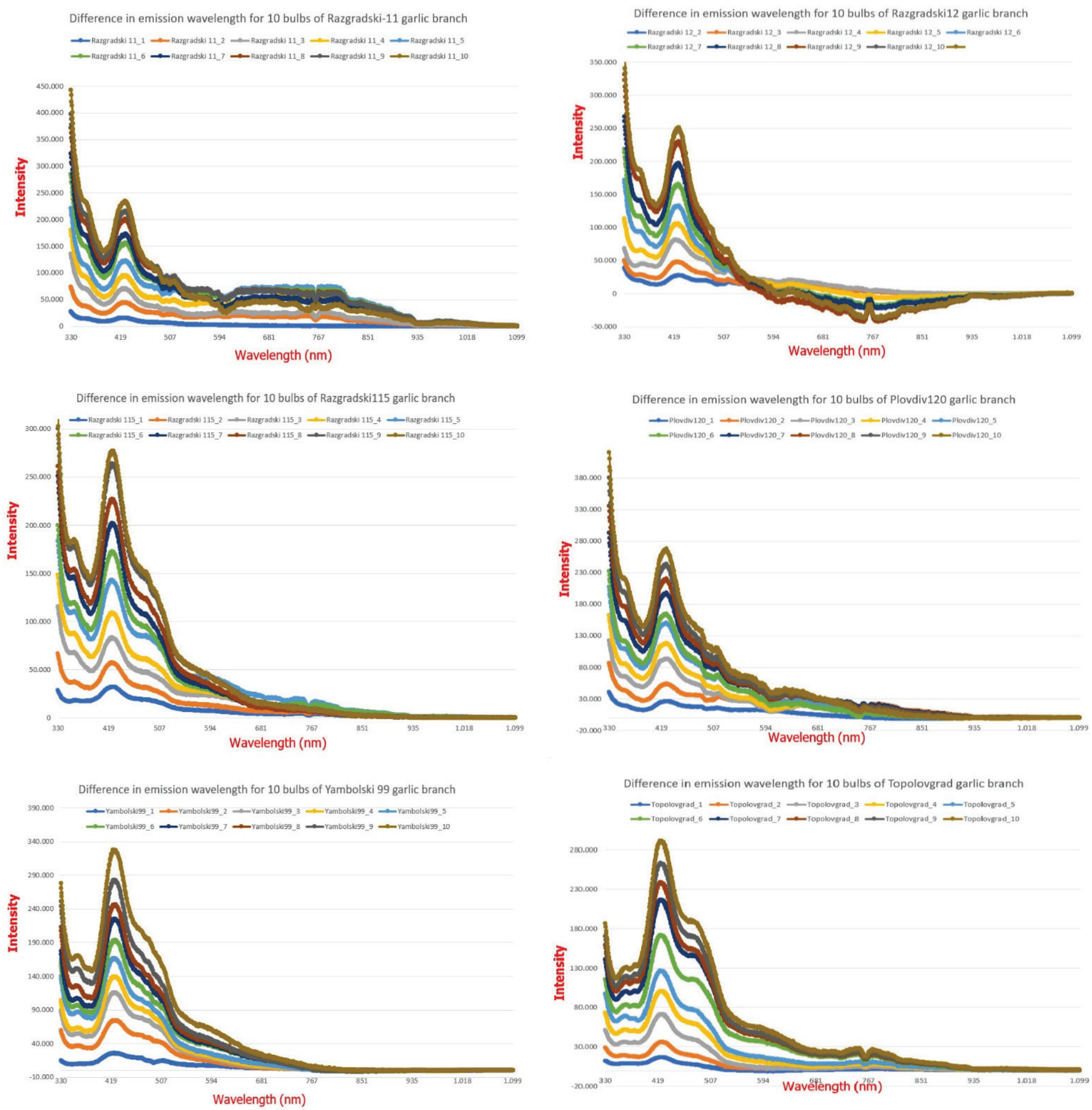

Figure 4 Difference in emission wavelength for 10 bulbs of a garlic branch

2.3 Separating Garlics with Machine Learning Methods

Each bulb of a specific branch of garlic reacts specifically, according to its cell-morphological and bacterial composition, to irradiation with ultraviolet light, correspondingly, it exhibits a unique spectral distribution characterized by a specific wavelength and intensity level immediately after recultivation. This is due to its organic and inorganic composition and its cell-morphological composition. A difference in the emission fluorescence signal of the different branches is clearly observed. Fluorescence spectroscopy can be successfully applied as a rapid tool to establish the origin of unknown bulbs. By tracking signal intensity, one can monitor the stability of a branch and its common blacks with other branches. In this study, 8118×11 fluorescent spectroscope dataset was created by taking the fluorescent spectroscopy data of ten bulbs of a specific garlic branch for each garlic variety. The fluorescence spectroscope graphic of ten onions from a bulbs garlic branch for each garlic variety is shown in Fig. 4.

The fluorescent spectroscopic data measured for each garlic species were used to construct a machine learning model for class differentiation of garlic cultivars. These models have been developed using 10 folds cross validation mode and ML algorithms to make the classification and analysis process more objective and free from randomness. In the 10 folds cross validation process, the data set is divided into 10 equal parts, nine of which are used for training and one for testing. By repeating this process with 10 turns, the average accuracy calculation is made by using all the data in both training and testing. Fig. 5 shows the cross validation process used in this study.

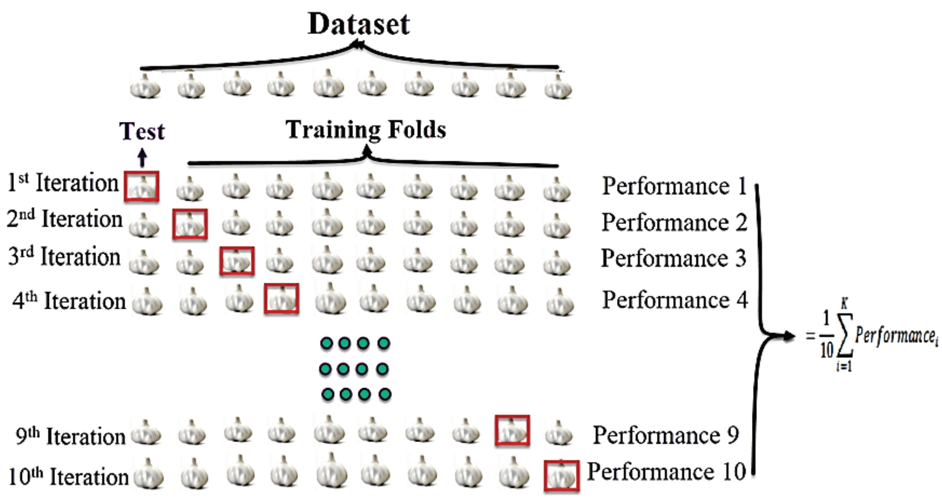

Figure 5 *k*-folds Cross-Validation

Because of the training and testing processes, Fine Tree, Quadratic Discriminant, Naive Bayes, Cubic Support Vector Machine (SVM), weighted KNN, wide Nural Network and logistic regression kernel models were selected as the algorithms providing the most satisfactory results. Fig. 6 shows the confusion matrix for dual class confusion matrix and multi class classification [27]. In each model, confusion matrices, accuracy, recall, specificity, F1-Score, Precision, and Matthews correlation coefficient (MCC) values were determined according to Eqs. (1)-(6) [28].

		Predicted Class	
		Pozitif (P)	Negative (N)
Actual Class	Pozitif (P)	TP	FN
	Negative (N)	FP	FP

(a)

		Predicted Class			
		C_1	C_2	....	C_N
Actual Class	C_1	$C_{1,1}$	FP	....	$C_{1,N}$
	C_2	FN	TP	....	FN
	...	...	...	....	...
	C_N	$C_{N,1}$	FP	...	$C_{N,N}$

(b)

Figure 6 Confusion matrix examples. (a) Binary classification problem confusion matrix. (b) Multiclass classification problem confusion matrix.

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN} \times 100, \tag{1}$$

$$Recall = \frac{TP}{TP+FN} \times 100, \tag{2}$$

$$Specificity = \frac{TN}{TN+FP} \times 100, \tag{3}$$

$$F1-Score = 2 \times \frac{Sensitivity \times Precision}{Sensitivity + Precision} \times 100, \tag{4}$$

$$Precision = \frac{TP}{TP+FP} \times 100, \tag{5}$$

$$Mcc = \frac{TP \times TN - FP \times FN}{\sqrt{(TP+FP)\times(TP+FN)\times(TN+FP)\times(TN+FN)}} \times 100. \tag{6}$$

In the study, the hyperparameter settings of each model were updated and the parameter was updated for optimum classification accuracy. Because of this, the performance metrics of the classification accuracy obtained were calculated and the models were compared.

3 RESULTS AND DISCUSSION

In this study, machine learning techniques Fine Tree, Quadratic Discriminant, Naive Bayes, Cubic Support Vector Machine (SVM), weighted KNN, wide Nural Network and logistic regression kernel models were used in the separation and classification of garlic varieties. The implementation of these models was carried out using Matlab R2022b software on a performance laptop with Intel Core i7-10750H-2.60 GHz CPU, 32 GB RAM 2.93 GHz, NVIDIA GeForce GTX 1650 Ti 4 GB and 500 GB NVMe2 SSD HDD. Classification of fluorescent spectroscopic data measured from whole garlic was performed with 10 folds cross validation using standard parameters of machine learning. The confusion matrix results of the classification results obtained by machine learning methods using standard parameter values are given in Fig. 7.

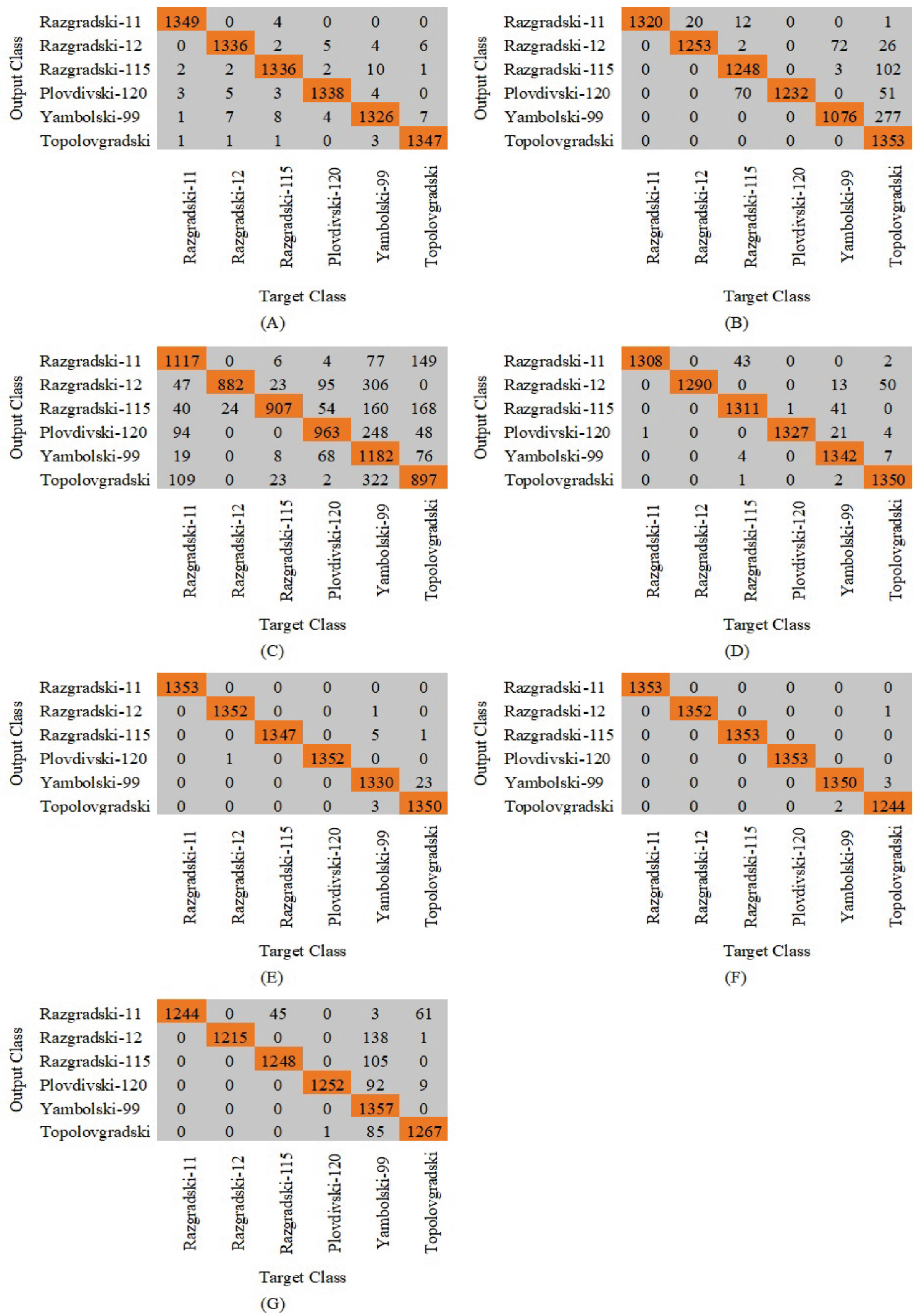

Figure 7 The confusion matrix results of the classification results obtained by machine learning methods using standard parameter values: A) Fine Tree Confusion Matrix, B) Quadratic Discriminant Confusion Matrix, C) Naive Bayes Confusion Matrix, D) Cubic SVM Confusion Matrix, E) Weighted KNN Confusion Matrix, F) Wide NN Confusion Matrix, G) LRK Confusion Matrix

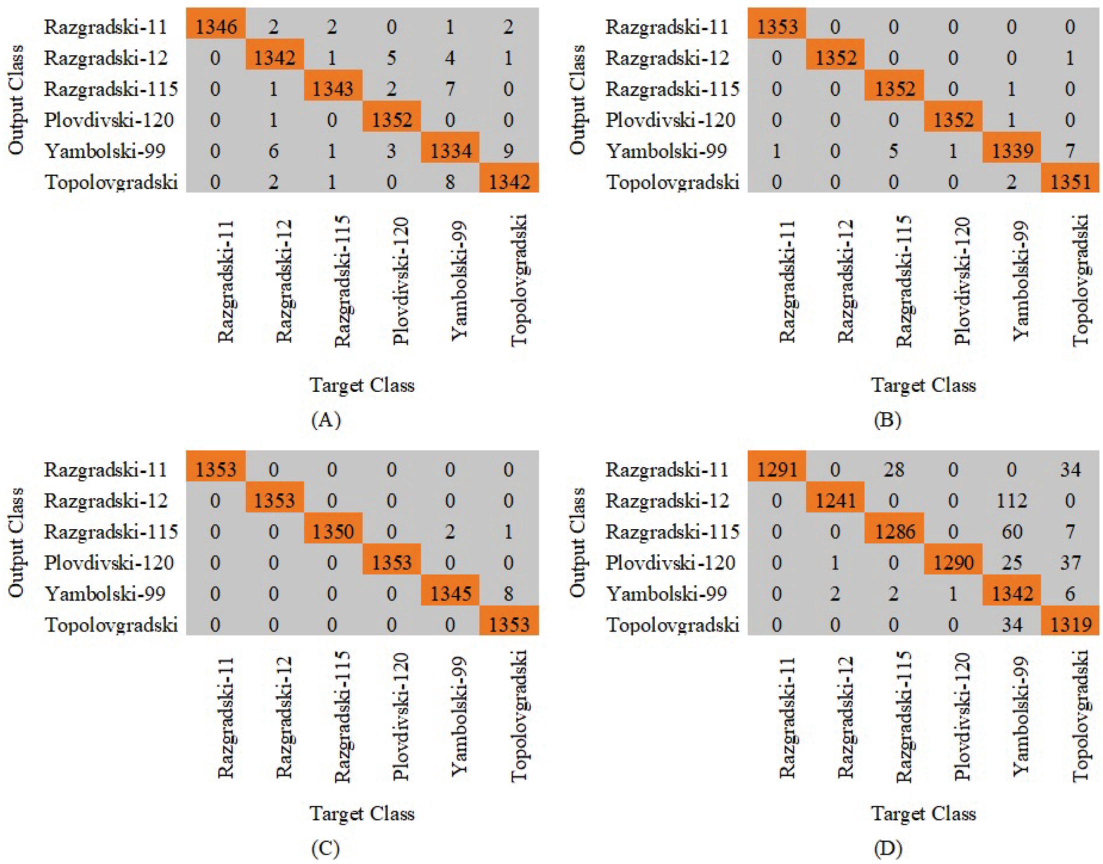

Figure 8 The confusion matrix results of the classification results obtained by machine learning methods using hyper parameter values: A) Fine Tree Confusion Matrix, B) SVM Confusion Matrix, C) Weighted KNN Confusion Matrix, D) LRK Confusion Matrix

The confusion matrix results of the classification results obtained by machine learning methods using hyper parameter values are given in Fig. 8. The accuracy rates of the models obtained in the classification of garlic varieties with the default parameters Fine Tree, Quadratic Discriminant, Naive Bayes, Cubic Support Vector Machine (SVM), weighted KNN, wide Nural Network and logistic regression Kernel (LRK) were 98.9%, 92.2%, %, respectively. 73.3%, 97.7%, 99.6%, 99.9% and 93.4%. Performance metrics obtained from the confusion matrix of the models are given in Tab. 1.

Table 1 Classification performance metrics using standard Parameter values

Model	Accuracy	Recall	Specificity	F1-Score	Precision	Matthews correlation coefficient (MCC)
Fine Tree	98.94	98.94	99.79	98.94	98.94	98.73
Quadratic Discriminant	92.17	92.17	98.43	92.33	93.39	91.09
Naive Bayes	73.27	73.27	94.65	74.00	78.20	69.93
Cubic SVM	97.66	97.66	99.53	97.67	97.74	97.22
Weighted KNN	99.58	99.58	99.92	99.58	99.58	99.50
Wide NN	99.93	99.93	99.99	99.93	99.93	99.91
LRK	93.36	93.36	98.67	93.59	94.56	92.53

The performance metrics obtained from the confusion matrix according to the optimized hyper parameter values of the models are given in Tab. 2. Standard parameters and optimized hyper parameters of the models are given in Tab. 3.

Table 2 Classification performance metrics using the optimum Parameter values of the models

Model	Accuracy	Recall	Specificity	F1-Score	Precision	Matthews correlation coefficient (MCC)
Fine Tree	99.27	99.27	99.85	99.27	99.27	99.13
Cubic SVM	99.77	99.77	99.95	99.77	99.77	99.72
Weighted KNN	99.86	99.86	99.97	99.86	99.87	99.84
LRK	95.7	95.70	99.14	95.77	96.12	95.01

In this study, in the first stage, the data set created from the fluorescent spectroscopic data of garlic images was classified using innovative models in machine learning techniques. Classification by combining non-destructive fluorescent spectroscopic techniques and artificial intelligence methods may be useful to use this method in practice. In the second stage, the parameters of the models were changed and the models were classified by machine learning methods by updating the parameters in order to reach the optimum classification accuracy. It was observed that the classification performance of Fine Tree, Cubic SVM, Weighted KNN, LRK models increased compared to standard parameters. With the performance values obtained, it is seen that garlic species can be classified by machine learning techniques using fluorescence spectral data.

Table 3 Standard and optimized hyper parameter values

Standard Model Parameters	Optimized Hyper Parameters
Fine Tree	Fine Tree
Maximum number of splits: 100 Split Criterion: Gini's Diversity index Surrogate Decision splits: Off	Maximum number of splits: 100 Split Criterion: Twoing rule Surrogate Decision splits: On, using a maximum of 10 surrogates
Cubic SVM	Cubic SVM
Kernel Function: Cubic Box constraint level: 1 Kernel Scala Mode: Auto Multiclass Method: One-vs-One Standardize Data: Yes	Kernel Function: Cubic Box constraint level: 6 Kernel Scala Mode: Auto Multiclass Method: One-vs-All Standardize Data: Yes
Weighted KNN	Weighted KNN
Number of Neighbours: 10 Distance metric: Euclidean Distance weight: Squared inverse Standardize data: Yes	Number of Neighbours: 10 Distance metric: Correlation Distance weight: Inverse Standardize data: Yes
LRK	LRK
Learner: Logistic Regression Number of expansion dimensions: Auto Regularization strength (lambda): Auto Kernel Scala: Auto Multiclass Method: One-vs-One Iteration limit: 1000	Learner: Logistic Regression Number of expansion dimensions: Auto Regularization strength (lambda): Auto Kernel Scala: Auto Multiclass Method: One-vs-All Iteration limit: 1000

4 CONCLUSION

The study involved a new approach combining fluorescence spectroscopy and traditional machine learning algorithms to distinguish garlic varieties. The procedure, performed by precise parameter tuning to improve the success of traditional machine learning methods, was innovative against the background of existing literature for garlic quality evaluation. Machine learning models built based on spectroscopic data allowed six different types of garlic to be classified with up to 99.93% accuracy. The most effective algorithms in the conducted study were the Wide NN classifier. It was observed that the classification performance of Fine Tree, Cubic SVM, Weighted KNN, and LRK classifiers increased in the classification process with parameter adjustment.

Future studies may include other spectroscopic techniques in studies of garlic cultivar classification or discrimination of species, cultivars and breeding lines, as well as various aspects of garlic seed quality assessment to be used as garlic seeds.

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