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Practical applications of neural network with Kolmogorov-Arnold layers in spectral analysis

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Abstract

The application of a neural network based on the CNN-KAN architecture for the automated analysis of spectroscopic data is presented. The study focuses on issues related to food quality assessment and the detection of different types of plastics used in packaging. The results demonstrate that the CNN-KAN architecture that combines convolutional and Kolmogorov-Arnold layers can be successfully applied to both binary and multiclass classification tasks, including scenarios involving datasets with a limited number of samples and/or low-resolution spectra. The study encompasses a range of practical applications, including the detection of purée samples adulterated with less expensive ingredients, the recognition of coffee species, the classification of plastic polymer samples, and the detection of ethanol level in beverages without the need to open the bottle.

Keywords: deep neural network, Kolmogorov-Arnold layers, IR spectra, detection of food adulteration, plastic polymer classification

1 Introduction

In recent years, machine learning (ML) and artificial intelligence (AI)-based solutions have gained increasing popularity. In particular, generative AI, especially solutions based on so-called large language models (LLMs) (e.g., ChatGPT), has become widely adopted and attracted significant attention [1]. The rapid development of ML applications is also evident in the field of physical chemistry. Neural networks are being used for molecular modeling [2], investigating the structure and thermodynamics of nanoclusters [3], addressing problems in heterogeneous catalysis [4], and many other scientific applications [5].

ML is also used for the automated analysis of FTIR spectra, including, among other applications, the detection of functional groups. Enders et al. [6] presented a convolutional neural network for the detection of 17 functional groups based on FTIR spectral images. Fine et al. [7] proposed a method for functional group detection using both FTIR spectra and mass spectrometry data, employing autoencoders and multilayer perceptrons. Doan et al. [8] introduced a transformer-based architecture for functional group detection from FTIR spectra, while more recently, in study by Öncü and Kızıllhan [9], a deep neural network based on the YOLOv8n framework for the same task was described.

In our previous article [10], we presented a set of binary classifiers for detecting 22 functional groups from FTIR spectra based on a convolutional neural network with Kolmogorov-Arnold layers (CNN-KAN). A key feature of this approach is that, unlike the methods described in e.g. Refs. [6] and [9], it operates directly on spectra represented as numerical vectors rather than on spectral images. In Ref. [10], we demonstrated that incorporating Kolmogorov-Arnold layers into the neural network significantly improves prediction performance of the classifier. Furthermore, using the SHAP framework [11], we showed in Ref. [12] that the predictions made by the CNN-KAN network are based on reliable and chemically meaningful evidences. The SHAP framework identified the spectral regions containing peaks characteristic of the corresponding functional group as the most important contributors to the predictions of CNN-KAN classifiers.

In this article, we aim to demonstrate that the CNN-KAN architecture can also be successfully applied to other problems related to the automation of FTIR spectra analysis, or even more general, in optical spectra analysis. We decided to focus on issues related to food quality assessment and the identification of different types of plastics commonly used in the production of packaging. In particular, we show that CNN-KAN performs well on spectra acquired at lower spectral resolution, can be effectively applied to problems with relatively small or imbalanced training datasets, and is also capable of handling multiclass classification tasks with high effectiveness.

Furthermore, this article demonstrates that our network architecture is applicable not only to fundamental scientific tasks, such as the identification of functional groups from FTIR spectra, but also to a variety of practical spectroscopy applications. We decided to focus on issues related to food quality assessment and the identification of different types of plastics commonly used in the production of packaging. In our experiments, we analyzed the following four problems: detection of fruit purées adulterated with less expensive ingredients, recognition of coffee species, plastic polymer

classification and noninvasive detection of alcohol concentration without opening the bottle of beverage.

2 Methodology

2.1 CNN-KAN architecture

The CNN-KAN architecture has been described in detail elsewhere [10] therefore, in this section we focus only on its most important characteristics related to the presence of Kolmogorov-Arnold layers. Detailed information on the principles of operation of neural networks (including convolutional neural networks) can be found, for example, in Ref. [13].

Figure 1 compares a neuron used in conventional fully connected layers of a multilayer perceptron network (Part A) with the neurons that constitute Kolmogorov-Arnold layers (Part B). In the case of traditional neurons, the output is obtained by applying a nonlinear activation function (e.g., ReLU or sigmoid) to the weighted sum of the input signals, where the input weights are learned during the training process.

In contrast, the operation of neurons in Kolmogorov-Arnold layers is based on the Kolmogorov-Arnold representation theorem [14], which states that any continuous multivariate function can be represented as a finite sum of univariate functions. During training, for each input of a Kolmogorov-Arnold neuron, the parameters of an individual univariate function (approximated using a spline function) are learned independently. The neuron's output is then computed as the sum of the values produced by these univariate functions. Unlike conventional neurons, Kolmogorov-Arnold neurons do not employ a nonlinear activation function. Instead, nonlinearity is introduced through the learned nonlinear univariate functions applied individually to each input variable.

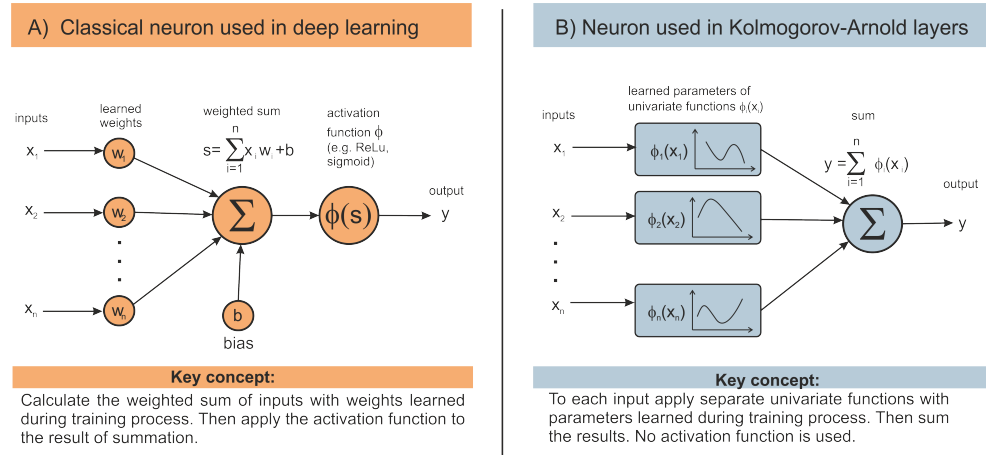


Fig. 1 Comparison of a conventional neuron used in multilayer perceptrons and a neuron from a Kolmogorov-Arnold layer.

Table 1 Overview of the datasets used in this study

Dataset	Strawberry purée adulteration	Coffee species recognition	Plastic polymer classification	Noninvasive detection of ethanol level
Number of classess	2	2	6	4
Number of samples	613 train 370 test	28 train 28 test	3000 total	504 train 500test
Spectrum length	235	286	3776	1751
Is balanced	No	Yes	Yes	Yes
Reference	[15]	[16]	[17]	[18]

2.2 Description of datasets

To demonstrate the applicability of the CNN-KAN architecture to different classes of problems in spectral analysis, four publicly available datasets were selected. Detailed information about the datasets are summarized in Table 1.

The three datasets [15, 16, 18] used in this study are part of a larger collection of benchmark datasets [19] developed by researchers at the University of California, Riverside (UCR) for evaluating and benchmarking ML models.

2.2.1 Strawberry purée adulteration

The first dataset [15] is associated with a real-world food fraud (economically motivated adulteration) problem involving the adulteration of food products by replacing a more expensive ingredient with a significantly cheaper alternative. Specifically, the dataset concerns the adulteration of strawberry purée by adding purées derived from less expensive fruits (*e.g.* apples) or other ingredients (*e.g.* sugar). This task is formulated as a binary classification problem, where the ML model must determine whether a fruit purée was produced exclusively from strawberries or whether it contains admixtures originating from other fruits or ingredients. The FTIR spectra in this dataset were acquired at relatively low spectral resolution, with each spectrum consisting of only 235 measurement points corresponding to the wavenumber range of 899-1802 cm^{-1} . The dataset contains a total of 983 labeled spectra and was originally divided into a training set (613 spectra) and a test set (370 spectra). The same train-test split was adopted in this study. Importantly, both the training and test sets are imbalanced. Approximately 64.3% of the samples correspond to adulterated strawberry purées containing additional fruit ingredients, whereas only about 35.7% represent authentic purées produced exclusively from strawberries. To mitigate the challenges associated with class imbalance, the Synthetic Minority Over-sampling Technique (SMOTE) [20] was applied independently both to train as well as test dataset. It is worth emphasizing that applying the SMOTE to the test set may negatively affect the comparability of the results obtained in this study with those reported in studies in which SMOTE was not applied.

2.2.2 Coffee species recognition

The second dataset analyzed in this study is related to the problem of classifying two coffee species, Robusta and Arabica, based on FTIR spectra [16]. This dataset contains a very small number of samples and was included in the analysis to demonstrate that advanced ML methods - particularly the neural network based on CNN-KAN architecture - can often be successfully applied even when only limited data are available. The dataset includes predefined training and test sets, each consisting of 28 samples, and both sets are balanced. Each sample is represented by a FTIR spectrum comprising 286 data points, recorded over the spectral range of 800-1900 cm^{-1} . In our experiments with this dataset, we decided to preserve the original split into the training and test sets. We chose not to transfer samples from the test set to the training set, as the test set is already very small, and further reducing its size would negatively affect the reliability of the evaluation results.

2.2.3 Plastic polymer classification

The third dataset [17] addresses a multiclass classification problem. The task is to determine the type of plastic polymer from which the analyzed sample is made based on its FTIR spectrum. Each sample belongs to one category corresponding to the most common synthetic plastic polymers used in industry and also in everyday products: polyethylene terephthalate (PET), high-density polyethylene (HDPE), polyvinyl chloride (PVC), low-density polyethylene (LDPE), polypropylene (PP), and polystyrene (PS). The dataset is balanced and consists of 3000 labeled FTIR spectra, with 600 spectra for each plastic polymer category. Each spectrum contains 3776 points. For this dataset, no predefined training/test split was provided. Therefore, we randomly divided the dataset, allocating 80% of the samples to the training set and the remaining 20% to the test set.

2.2.4 Noninvasive detection of ethanol level

The fourth dataset considered in this study is also related to food adulteration. It addresses the problem of determination of the alcohol concentration in the beverage based on the recorded spectra, without the need to open the bottle [18]. Consequently, this approach can be used for rapid, non-destructive screening to identify bottles that exhibit content deviations and should, therefore, be subjected to more detailed analysis using more accurate methods. The dataset contains four ethanol concentration levels: 35%, 38%, 40%, and 45% [18]. It is associated with a series of studies conducted by Anthony Bagnall’s research group at the University of East Anglia on the detection of counterfeit alcoholic beverages [18, 21, 22]. Unlike the other datasets discussed in this article that are based on FTIR spectra, this dataset consists of visible and near-infrared (VIS-NIR) spectra acquired using the simple grating spectrometer StellarNet BLACKComet-SR. Owing to its simplicity and portability, this instrument is well suited for rapid measurements, for example, at points of sale. The dataset is divided into a training set containing 504 spectra and a test set containing 500 spectra. Each spectrum consists of 1751 measurement points. Both the training and test sets are class-balanced. An important characteristic of this dataset is that the recorded spectra

may be influenced not only by the alcohol concentration but also by the type of bottle. The dataset was designed so that the bottles included in the test set differ from those used in the training set. For this reason, the experiments presented here preserve the original training - test split, even though the comparable size of both subsets and relatively small number of samples in the training dataset made it tempting to transfer some samples from the test set to the training set.

3 Results

In the conducted experiments, the accuracy, specificity, and recall metrics obtained by the neural networks based on CNN-KAN architecture were compared with the corresponding metrics achieved by a neural networks based on so called "simple CNN" architecture. In the simple CNN architecture, the convolutional layers were followed by fully connected layers composed of conventional neurons. For each problem analyzed in this article, the convolutional part of the simple CNN architecture was identical to that of the CNN-KAN network. To ensure a fair comparison, the number of conventional neurons in the simple CNN was selected so that the total number of trainable parameters matched that of the CNN-KAN architecture. Moreover, for each of the analyzed problems, the neural network hyperparameters (e.g., the number of training epochs, batch size, learning rate) were identical for both the CNN-KAN and simple CNN architectures. The detailed information about used architecture and hyperparameters can be found in Table 2. All neural networks described in this article were trained using the AdamW optimizer [23] and were implemented in Python using the PyTorch [24] deep learning framework. Neural networks with KAN layers were built using the *efficient KAN* library [25].

Training neural networks inherently involve a degree of randomness arising, among other factors, from the random initialization of network weights and the random order in which training samples are presented during the learning process. Therefore, to obtain more reliable results, we performed 14 independent training runs for each dataset. This approach allowed us to report the average values of the evaluation metrics (accuracy, precision, and recall; the precise definitions will be given below) together with their standard deviations. Considering that neural network training inherently involves randomness, we introduced an additional procedure that was applied to each of the problems analyzed in this study. From the set of trained models used for the subsequent evaluation of training performance, we consistently discarded the four worst-performing models. More specifically, we excluded the models with the lowest accuracy on the training set: the two worst-performing models for the CNN-KAN architecture and the two worst-performing models for the simple CNN architecture. The discarded runs were not included in the statistics presented in Table 3 or in the plots shown in Figure 2.

For binary classifiers, we used the standard definitions of the accuracy (*acc*), specificity (*spec*), and recall (*rec*) metrics throughout this article. Specifically,

$$acc = \frac{TP + TN}{TP + TN + FP + FN},$$

Table 2 Overview of the neural networks architectures used in this study

CNN-KAN architecture				
Dataset	Strawberry purée adulteration	Coffee species recognition	Plastic polymer classification	Noninvasive detection of ethanol level
Total number of parameters	1471	2700	34308	27240
Convolutional part	Conv1D (10) Conv1D (10) Conv1D (10)	Conv1D (10) Conv1D (10) Conv1D (10)	Conv1D (16) Conv1D (8) Conv1D (4)	Conv1D (20) Conv1D (20) Conv1D (10)
Ending part	KAN (2) KAN (1)	KAN (2) KAN (1)	KAN (6) KAN (6)	KAN (4)

Simple CNN architecture				
Dataset	Strawberry purée adulteration	Coffee species recognition	Plastic polymer classification	Noninvasive detection of ethanol level
Total number of parameters	1471	2811	35354	27644
Convolutional part	Conv1D (10) Conv1D (10) Conv1D (10)	Conv1D (10) Conv1D (10) Conv1D (10)	Conv1D (16) Conv1D (8) Conv1D (4)	Conv1D (20) Conv1D (20) Conv1D (10)
Ending part	LReLU (6) LReLU (3) Sigmoid (1)	LReLU (20) LReLU (5) Sigmoid (1)	LReLU (60) LReLU (20) Sigmoid (6)	LReLU (40) LReLU (8) Sigmoid (4)

Hyperparameters common for both architectures				
Dataset	Strawberry purée adulteration	Coffee species recognition	Plastic polymer classification	Noninvasive detection of ethanol level
Epochs	50	50	80	400
Batch size	64	5	64	256
Learning rate	$1.0 \cdot 10^{-2}$	$1.0 \cdot 10^{-2}$	$1.0 \cdot 10^{-3}$	$5.0 \cdot 10^{-3}$
Weight decay	$5.0 \cdot 10^{-3}$	$5.0 \cdot 10^{-3}$	$1.0 \cdot 10^{-2}$	$5.0 \cdot 10^{-4}$
Lambda LR	0.9	0.9	0.99	0.995

$$spec = \frac{TN}{TN + FP},$$

$$rec = \frac{TP}{TP + FN},$$

where TP , TN , FP and FN denote the number of true positive, true negative, false positive and false negative predictions, respectively.

Defining these metrics for multiclass classifiers is somewhat more complex. In multiclass classification one of the simplest metrics used to assess a classifier’s predictive performance is accuracy, defined as the ratio of correctly classified samples ($TP + TN$) to the total number of predictions. This metric is defined analogously to the binary classification case. The definition of the remaining metrics is more complicated. There are at least two common approaches to reporting specificity and recall (or other similar metrics) for multiclass classifiers. The first approach is to report metrics separately

for each class. In this case, specificity for class A is defined as

$$spec = \frac{TN_A}{TN_A + FP_A},$$

while recall is defined as

$$rec = \frac{TP_A}{TP_A + FN_A},$$

where TP_A and TN_A denote the number of true positive and true negative predictions belonging to A class, respectively, whereas FP_A and FN_A denote false positive and false negative predictions for A class, respectively. The second approach is to compute the recall and precision for each class individually and then report their average values across all classes. This approach is particularly appropriate when the dataset is balanced, as is the case for the datasets considered in this study so the approach was used in data analysis.

3.1 Strawberry purée adulteration dataset

The problem under investigation is characterized by a relatively short input feature vector (235 features, the smallest among all the datasets considered) and an imbalanced dataset. To address the class imbalance, as mentioned above, the SMOTE technique was applied independently to both the training and test subsets. The neural network architectures used in this study are relatively simple. Both the CNN-KAN and the simple CNN models contain 1,471 trainable parameters.

The averaged training results are presented in Part A of Table 3, while the detailed results for all trials are collected in Appendix A. As one can see, for both the training and test sets, all averaged performance metrics are higher for the CNN-KAN architecture than for the simple CNN architecture, although the differences are not particularly large. For example, the main test set metrics - accuracy, averaged over 10 independent runs, is 1.16 percentage points higher for the CNN-KAN architecture than in the case of simple CNN architecture. The overall performance metrics for both architectures achieved on this dataset are high, indicating that the models provides highly accurate predictions. Figure 2A shows the box plots for test set accuracies for the CNN-KAN and the simple CNN architectures. The points overlaid on the box plots represent the results of individual trials.

3.2 The coffee species recognition dataset

The dataset analyzed in this subsection is characterized by a very small number of samples (28 in the training set and 28 in the test set). The training results obtained for the CNN-KAN and simple CNN architectures are summarized in part B of Table 3, which reports the average values of the accuracy, specificity, and recall metrics for both the training and test sets. Detailed results for individual trials are reported in Appendix B. Additionally, Figure 2B presents the accuracy values obtained for the test set as a box plot, whereas points overlaid on the box plots represent the results of individual trials.

Table 3 Average values of the accuracy (*acc*), specificity (*spec*), and recall (*rec*) metrics over 10 trials for models based on the CNN-KAN and simple CNN architectures, evaluated on the training and test sets. All values are given as percentages. Detailed data used to calculate the averages are provided in Appendices A-D.

Part A. Results for strawberry purée adulteration dataset						
	Training dataset			Test dataset		
Architecture	<i>acc</i>	<i>spec</i>	<i>rec</i>	<i>acc</i>	<i>spec</i>	<i>rec</i>
CNN-KAN	97.4	98.5	96.2	93.7	95.9	91.5
Simple CNN	96.2	97.2	95.2	92.5	94.9	90.2

Part B. Results for coffee species recognition dataset						
	Training dataset			Test dataset		
Architecture	<i>acc</i>	<i>spec</i>	<i>rec</i>	<i>acc</i>	<i>spec</i>	<i>rec</i>
CNN-KAN	100.0	100.0	100.0	96.8	99.3	93.9
Simple CNN	99.6	100.0	99.3	95.7	99.3	91.5

Part C. Results for plastic polymer classification dataset						
	Train dataset			Test dataset		
Architecture	<i>acc</i>	<i>spec</i>	<i>rec</i>	<i>acc</i>	<i>spec</i>	<i>rec</i>
CNN-KAN	94.8	99.0	94.7	94.5	98.9	94.79
Simple CNN	88.9	97.8	88.8	88.4	97.7	88.7

Part D. Results for noninvasive detection of ethanol level dataset						
	Train dataset			Test dataset		
Architecture	<i>acc</i>	<i>spec</i>	<i>rec</i>	<i>acc</i>	<i>spec</i>	<i>rec</i>
CNN-KAN	92.4	97.5	92.4	72.2	90.8	72.3
Simple CNN	67.7	89.3	67.7	56.6	85.5	56.7

It should be noted that, due to the very small size of the test set, the accuracy values (as well as the other evaluation metrics) can assume only a limited number of discrete values. Consequently, the points in Figure 2B are arranged along horizontal lines.

The average evaluation metrics indicate that the CNN-KAN architecture provides better predictive performance than the simple CNN architecture. It can generally be concluded that both architectures achieved high predictive performance, with mean accuracy values exceeding 95%. The conducted analysis demonstrates that the CNN-KAN architecture can be successfully applied even to datasets containing a very small number of samples.

To maintain consistency, the metrics in the table 3 are rounded to one decimal place. It is worth noting that, in the case of coffee species classification, the test set is limited to only 28 samples. With such a small number of samples, the misclassification of a single sample affects the accuracy metric by 3.6%. Moreover, the metric values (e.g., accuracy) are rather strongly quantized, as can be seen in Figure 2B.

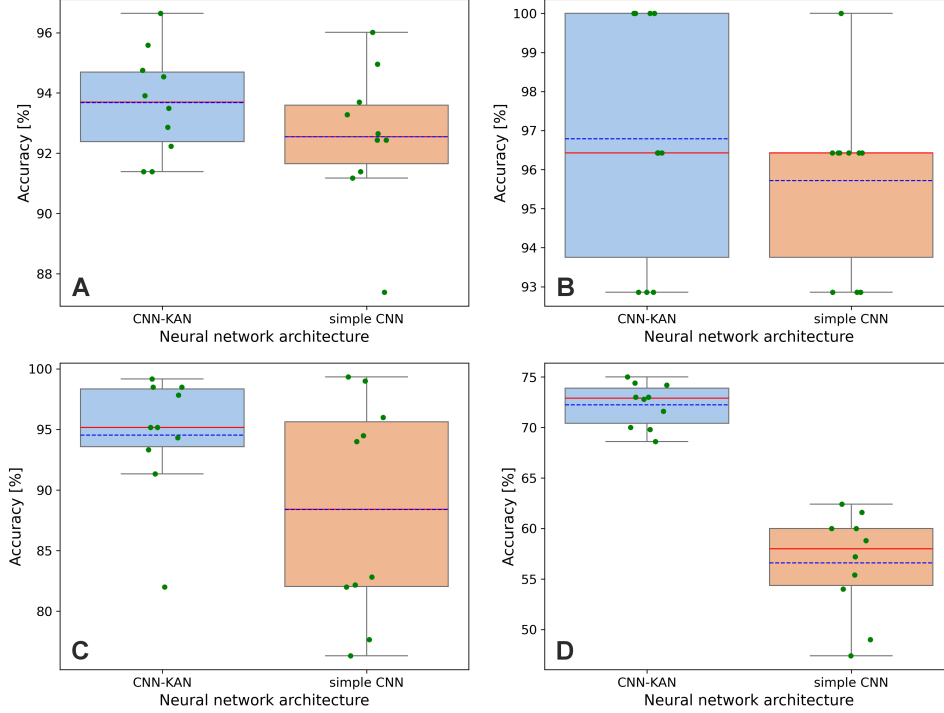


Fig. 2 Box plots showing the distribution of the accuracy metric for simple CNN and CNN-KAN neural network architectures on the test sets of the datasets analyzed in the article. Part A: strawberry purée adulteration dataset, part B: coffee species recognition dataset, part C: plastic polymer classification dataset, and part D: non-invasive detection of ethanol concentration in alcoholic beverages dataset). The green points indicate the accuracy values obtained in individual neural network training runs. The red lines inside the boxes represent the medians, while the blue dashed lines indicate the means (please note that in part A and for the simple CNN architecture in part C, these lines lie very close to each other). The upper and lower edges of each box correspond to the third and first quartiles of the distribution, respectively. The plots were generated using the boxplot function from the Seaborn library [26]. Details in text.

3.3 Plastic polymer classification dataset

Plastic polymer classification is an example of a multiclass classification problem. In this classification task each spectrum is assigned to exactly one of six classes. The dataset analyzed in this section has the largest input vector length (3776 elements), which results in increased neural network complexity. Both evaluated architectures comprised approximately 35000 trainable parameters. Part C of Table 3 presents the average values of accuracy, specificity, and recall obtained over 10 independent training runs for both examined architectures of neural network. Figure 2C presents the box plots for accuracy values obtained for the test set for both architectures. As in the Figure 2A and Figure 2B, the points represent the results of individual trials. Detailed results for each individual training run are collected in Appendix C. It should be noted that the specificity and recall values were calculated as averages across all six classes (details described at the beginning of Section 3). To visualize the performance of the

CNN-KAN model, Figure 3 shows the confusion matrix for the model obtained in one of the training runs. The confusion matrices for the remaining CNN-KAN training runs, as well as the results obtained with the simple CNN architecture, are reported in Appendix C.

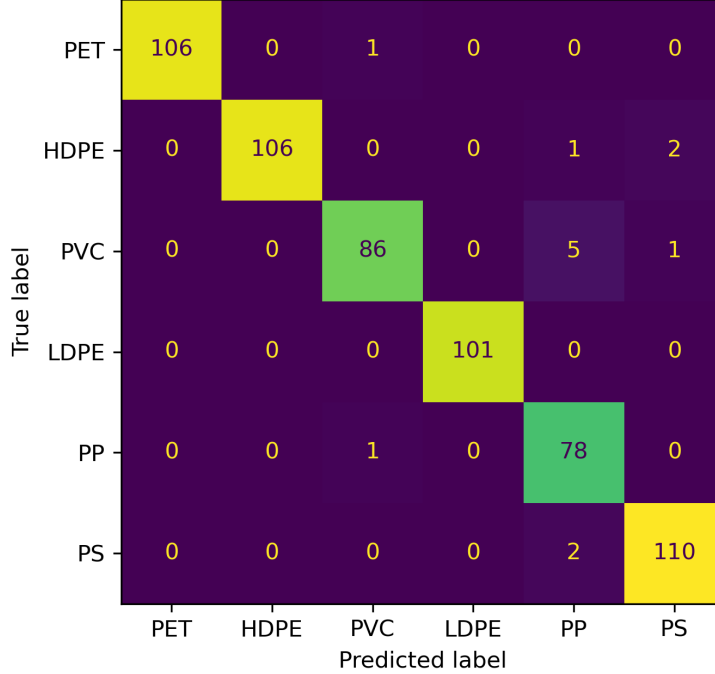


Fig. 3 Confusion matrix for the test set obtained using a representative neural network based on the CNN-KAN architecture for plastic polymer classification problem. Corresponding confusion matrices for all training runs are reported in Appendix C.

For this dataset, it is worth noting that the inferior performance of the simple CNN model is mainly due to its frequent misclassification of LDPE samples as HDPE. This can be readily observed in the confusion matrix for the training set, where the model incorrectly classified all spectra corresponding to the LDPE polymer. In contrast, this type of misclassification occurs less frequently in the CNN-KAN architecture.

3.4 Dataset for the noninvasive detection of ethanol level in alcoholic beverages

The dataset analyzed in this section represents another multiclass classification problem. Each spectrum is assigned to exactly one of the four possible alcohol concentrations in the analyzed sample. The spectra in the analyzed dataset consist of 1751 data points, while the evaluated ML models contain slightly over 27000 parameters. The average results obtained over 10 trials for the CNN-KAN and simple CNN

architectures are presented in Part D of Table 3. Detailed results, together with the confusion matrices for all runs, are collected in Appendix D. Figure 2D presents the box plots for accuracy values obtained for the test set for both architectures, where green points present results of individual trails.

This dataset proved to be the most challenging for training the neural networks, as the achieved performance metrics (e.g. test set accuracy) were considerably lower than those obtained for the other datasets. Nevertheless, for this dataset the CNN-KAN architecture clearly outperformed the simple CNN architecture. In particular, the average test set accuracy of the CNN-KAN model exceeded that of the simple CNN by 15.66 percentage points (72.24% vs. 56.58%).

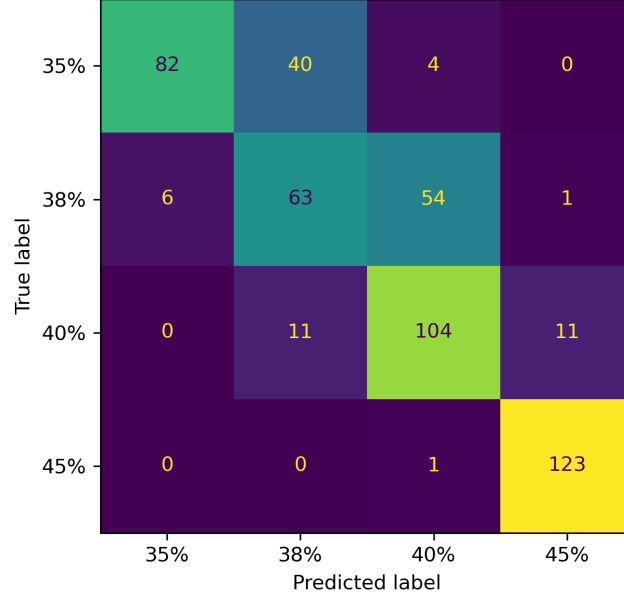


Fig. 4 Confusion matrix for the test set obtained using a representative neural network based on the CNN-KAN architecture for problem of noninvasive detection of ethanol level. Corresponding confusion matrices for all training runs are collected in Appendix D.

Additional insights can be obtained from the analysis of the confusion matrices. The confusion matrices for all runs are collected in Appendix D while Figure 4 presents an example of confusion matrix for the single CNN-KAN model evaluated on the test set. It can be observed that the prediction accuracy for the single class associated with 45% alcohol concentration is substantially higher than for the remaining concentration levels. This can be explained by the concentration values used in the study, namely 35%, 38%, 40%, and 45%. The class associated with 45% concentration of ethanol is clearly separated from the other three classes, whose concentration values are much closer to one another. This observation suggests that a classifier designed to distinguish only three concentration levels (35%, 40%, and 45%) would likely achieve substantially better predictive performance.

Although the overall prediction accuracy obtained for this dataset is relatively modest, it may still be sufficient for noninvasive screening applications. For example, the proposed method could be successfully used to identify bottles containing a very high alcohol concentration (45%).

4 Conclusions

This study demonstrates that a neural network architecture combining convolutional layers with Kolmogorov-Arnold layers (called in this article as CNN-KAN) can be successfully applied to the automatic analysis of spectroscopic data. We showed that the CNN-KAN architecture is capable of solving problems of varying complexity, including both binary and multiclass classification tasks, and performs well across datasets of different sizes. In particular, we demonstrated that the proposed architecture achieves satisfactory performance even when trained on extremely small datasets, such as the coffee species recognition dataset containing only 28 training samples.

The results further show that the predictive performance of the CNN-KAN architecture, measured in terms of accuracy, is comparable (for strawberry purée adulteration and coffee species recognition datasets) and even exceeds (for polymer classification and ethanol level detection datasets) that of a conventional convolutional neural network that consists of convolutional layers followed by several fully connected layers with leaky ReLU and sigmoid activation functions. Importantly, both architectures contained a comparable number of trainable parameters, ensuring a fair comparison.

The standard deviations of the obtained performance metrics for all dataset except the coffee species recognition dataset (details reported in Appendices A -D) were also considerably lower for the CNN-KAN architecture than for the corresponding simple CNN architecture. This indicates that the training process of the CNN-KAN network is more stable and produces more consistent and predictable results. The results obtained for the test subset of the coffee species recognition dataset show the opposite trend. Higher standard deviations of the performance metrics are observed for models based on the CNN-KAN architecture. This may be caused by the extremely small number of samples in both the training and test subsets of this dataset.

It should be emphasized, however, that the objective of this work was not to develop the most accurate predictive models possible. Achieving state-of-the-art performance would likely require combining the predictions of multiple classifiers using ensemble methods. Furthermore, we do not claim that the simple CNN architecture selected as the baseline in this study represents the optimal solution for the considered classification problems. For example, the relatively poor performance of the simple CNN on the noninvasive detection of ethanol level dataset motivated us to conduct additional experiments, which indicated that replacing the leaky ReLU activation functions in the two penultimate layers with SELU (Scaled Exponential Linear Unit) activation functions significantly improved the predictive performance of simple CNN architecture (for the modified architecture the average accuracy achieved on the test set was 62% instead of 57%).

The primary goal of this work was to demonstrate the usefulness of the CNN-KAN architecture and, more broadly, neural network architectures incorporating Kolmogorov-Arnold layers for solving a wide range of spectroscopic classification problems, in particular, to problems related to food quality assessment. We believe this is particularly relevant given the growing interest in neural networks based on Kolmogorov-Arnold layers in recent years [27–29] and, more broadly, in the use of deep learning methods in practical applications.

Supplementary information. The article includes the following supplementary materials:

- Appendix A - Detailed results for strawberry purée adulteration dataset. The file contains confusion matrices and performance metrics for individual runs.
- Appendix B - Detailed results for coffee species recognition dataset. The file contains confusion matrices and performance metrics for individual runs.
- Appendix C - Detailed results for polymer classification. The file contains confusion matrices and performance metrics for individual runs.
- Appendix D - Detailed results for noninvasive detection of ethanol level dataset. The file contains confusion matrices and performance metrics for individual runs.

Declaration of generative AI and AI-assisted technologies in the manuscript preparation process. During the preparation of this work the authors used the chatGPT in order to improve the language quality of the article. After using this tool, the authors reviewed and edited the content as needed. The authors take full responsibility for the content of the published article.

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