Computers and Electronics in Agriculture 235 (2025) 110354

Contents lists available at ScienceDirect

Computers and Electronics in Agriculture

journal homepage: www.elsevier.com/locate/compag

Review

A systematic review of explainable artificial intelligence for spectroscopic agricultural quality assessment

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ARTICLE INFO

Keywords:
Systematic review
Spectroscopic analysis
Machine learning
Agricultural quality
Explainable artificial intelligence

ABSTRACT

The introduction of complex machine learning models has greatly improved the accuracy and practical use of spectroscopic analyses in agriculture. However, users often struggle to understand how these models operate internally or how specific features contribute to the predictions. This lack of clarity can hinder innovation in agricultural spectroscopy, especially in selecting appropriate spectral wavelengths for domain specific applications or designing portable and low-cost devices. Therefore, the integration of Explainable Artificial Intelligence (XAI) techniques is essential to address these challenges in the agricultural sector. This review systematically examines recent advancements in XAI techniques and highlights their substantial effects on enhancing spectroscopic models for assessing the quality of agricultural and food products. This study also highlights current challenges and explores prospects, emphasizing how these innovative techniques can support more advanced and widely adopted applications within the agricultural industry.

1. Introduction

Agricultural quality assessment plays a crucial role in ensuring food safety, nutritional integrity, and the economic well-being of producers and consumers (Chuquimarca et al., 2024; Ghazal et al., 2024). As globalization expands the agricultural supply chain from farm to fork, complex environmental, economic, and demographic pressures increasingly impact product quality (Nugroho et al., 2021). Meeting the demands of a growing population and interconnected markets necessitates rigorous quality standards across every production stage to comply with international trade regulations, fulfill consumer expectations, and promote sustainable practices (Ahmed et al., 2023). The global agricultural testing (e.g., seeds, biosolids, water) market, valued at US dollar ($) 6.9 billion in 2024, is expected to grow at a compound annual growth rate (CAGR) of 7.2 % to reach $11.6 billion by 2030, with conventional methods continuing to hold the largest market share (Fig. 1). While conventional methods such as sensory evaluation, chemical analysis, and microbial testing are accurate, they are often labor-intensive, costly, and require specialized expertise, making them insufficient for high-throughput quality assessment (Elmasry et al., 2012; Kamruzzaman, 2023; Su et al., 2024). Consequently, these limitations highlight advanced, automated, and smart approaches for real-time quality assessment, consistently maintaining standards throughout the supply chain.

Spectroscopy has emerged as a powerful, smart, and nondestructive analytical tool for assessing agricultural and food product quality. Near Infrared (NIR), Fourier Transform Infrared (FTIR), Raman spectroscopy, and Hyperspectral Imaging (HSI) have been widely used for a range of parameters such as moisture content, nutrient composition, contaminant levels, texture, chemical composition, structural integrity, and quality control in various agricultural and food products (Ahmed et al., 2025a; Pasquini, 2018; Silva and Melo-Pinto, 2023; Sun et al., 2024; Zhu et al., 2023). Different artificial intelligence (AI) models, including machine learning and deep learning techniques, are used to predict target parameters in spectroscopic analysis (Hariharan et al., 2023; Liu et al., 2024; Partel et al., 2019; Shaikh et al., 2022a, Shaikh et al., 2022b). However, conventional spectroscopic models, often termed “black-box” models, face several limitations, primarily due to their complexity and lack of interpretability (Ahmed et al., 2025b; Dobbelaere et al., 2021). Despite their accuracy, the lack of transparency and explainability limits the industrial applications of spectroscopic techniques (Ahmed et al., 2025c; Cardoso Rial, 2024; Li et al., 2024). Such opacity hinders researchers’ ability to interpret and trust the results fully, emphasizing advanced explainable techniques to enhance analytical reliability and scientific understanding of spectroscopic models.

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https://doi.org/10.1016/j.compag.2025.110354
Received 17 January 2025; Received in revised form 24 March 2025; Accepted 26 March 2025
Available online 2 April 2025

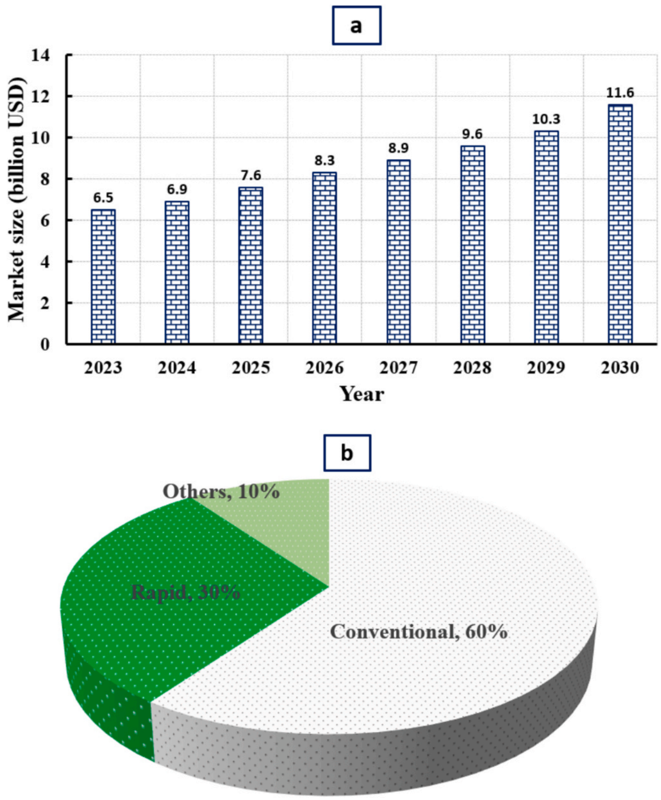

Fig. 1. Global agricultural testing market: a. Annual growth of market size in billion USD, b. agricultural testing by methods (CMI, 2025).

Explainable artificial intelligence (XAI) is an emerging technology that enhances transparency and trust by addressing interpretability challenges in complex AI-driven models (Abusitta et al., 2024; Hosain et al., 2024). Unlike conventional black-box models, XAI provides insights into the factors influencing predictions, which is important for robust model development, where interpretability ensures reliable, scientifically meaningful results (Ullah et al., 2024). Although relatively new in spectroscopic analyses, XAI is gaining popularity, with recent studies demonstrating its potential for spectroscopic model interpretation (Zhang and Yang, 2024). The XAI market is expanding rapidly as researchers and industry professionals explore its applications, driven by the growing demand for transparency and trust in AI systems. Its adoption spans multiple sectors, with healthcare leading at 43 % and food and agriculture collectively accounting for 12 %, highlighting XAI's increasing significance in these fields (Fig. 2).

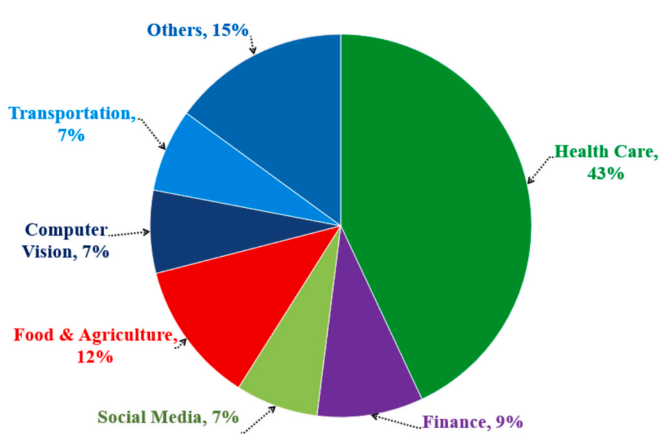

Fig. 2. Application domain of explainable artificial intelligence (Saranya and Subhashini, 2023).

Despite the recent advancements in spectroscopic techniques and machine learning, there is a notable gap in research consolidating the progress of explainable AI in agricultural quality assessment. While individual studies have explored various aspects of XAI in spectral analysis, including spectroscopy and HSI applications, a systematic framework that comprehensively examines the integration of XAI techniques in this domain remains lacking. Additionally, studies that address XAI for agricultural quality assessment are often dispersed across multiple subfields, lacking a cohesive synthesis that identifies trends, challenges, and research gaps. Although multiple reviews have been published on the use of XAI across various fields (Saranya and Subhashini, 2023; Angelov et al., 2021; Buyuktepe et al., 2023; Contreras and Bocklitz, 2024; Islam et al., 2022; Minh et al., 2022), a significant gap exists in the literature regarding its application in advancing agricultural quality assessment. To address this gap, this systematic review aims to analyze, synthesize, and categorize the existing literature on XAI methods in agricultural quality assessment. Specifically, the study highlights XAI's limitations, challenges, future directions, and potential to revolutionize smart and non-destructive agricultural quality assessment.

2. Research methodology

This section explains the Systematic Literature Review (SLR) method as guided by the PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) guidelines (Liberati, 2009; Page et al., 2021). PRISMA is used to summarize existing literature within a specific research area to derive final results. The protocol involves a four-phase flowchart: identification, screening, eligibility, and inclusion (Page et al., 2021). This structured process helps ensure that systematic reviews and *meta*-analyses are reported in a uniform and precise manner. While using this protocol aims to reduce biases in review studies, many reviews may still suffer from selective reporting of outcomes. Furthermore, using appropriate eligibility conditions and Boolean search terms across various databases can help filter out unrelated articles (Sokouti and Sokouti, 2018). In this study, an initial set of 72 articles was identified by searching bibliographic databases such as Scopus, IEEE Xplore, and Google Scholar. After screening the titles and abstracts, 27 articles were excluded. From the remaining 45 articles, 22 duplicates were removed, leaving 23 articles for in-depth analysis. Due to insufficient data and analysis in some articles, 6 more were excluded. Ultimately, 17 articles were included in this systematic review and analysis. This meticulous selection approach guaranteed a complete and unbiased evaluation of the current state and emerging trends in the research domain. Fig. 3 illustrates the stages of literature screening and selection according to the PRISMA protocol.

Fig. 4 displays a keyword cloud generated from 17 selected articles published between 2019 and 2024. This graphic highlights key terms based on their frequency and importance, with larger text sizes representing the most common topics in the field. The significant presence of terms like "Hyperspectral Imaging," "Spectroscopy," and "Explainable AI" indicates a shift toward advanced, nondestructive methods in agriculture. Similarly, the emphasis on "Deep Learning," "Machine Learning," and "Regression" reflects a strong focus on applied research aimed at improving computational techniques for assessing the quality of agricultural products. The keyword cloud effectively captures current trends and points out areas for future research, providing a clear overview of the field's development and technological environment.

3. XAI methods

XAI provides clear explanations for ML techniques, helping users understand, trust, and manage AI systems (Gunning et al., 2019). While an ML model can be explained, its interpretability mainly stems from its initial design (Barredo Arrieta et al., 2020). Although some linear and

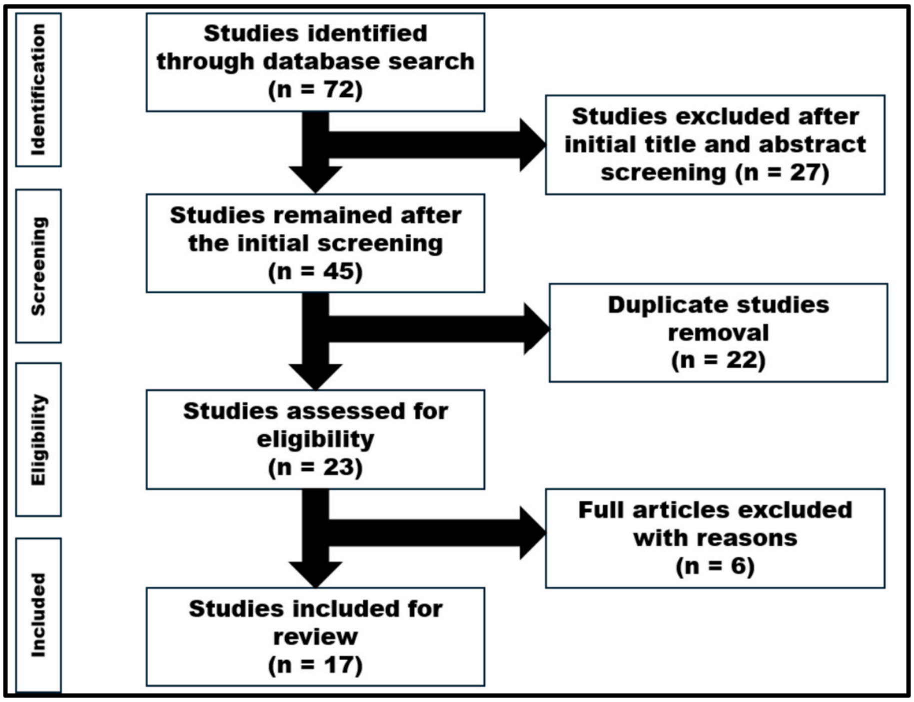

Fig. 3. PRISMA flowchart of study selection for the systematic review.

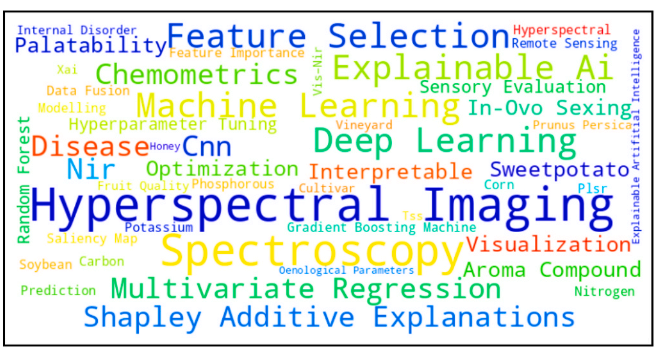

Fig. 4. Keyword cloud of frequent keywords in the relevant literature (2019–2024).

simple non-linear ML methods are interpretable due to their straightforward algorithmic structure, they do not offer explanations at the level of individual samples. Therefore, to enhance understanding, explainability often involves using post-hoc techniques, also referred to as post-modeling explainability. These techniques make models that are not initially interpretable more understandable. Most XAI applications focus on these post-hoc methods (Barredo Arrieta et al., 2020; Minh et al., 2022). The remaining sections will discuss XAI as mainly post-hoc methods. This section reviews and categorizes different XAI approaches, with a summary outlined in Table 1.

3.1. Feature-based methods

3.1.1. SHAP

SHAP (SHapley Additive exPlanation) is an important XAI method that analyzes the contribution of individual features in predictive models (Lundberg et al., 2020). The SHAP values come from cooperative game theory and measure each feature's impact on predictions by considering all possible feature combinations and their contributions (Shapley, 1953). Features that significantly affect predictions get higher importance rankings, shown through a feature importance plot that uses SHAP values. However, if an ML model is not additive, interpreting SHAP values can be unclear because the divisions of outcomes among features may not be independent (Angelov et al., 2021). Additionally, although SHAP is model agnostic, adapting the SHAP algorithm to all model types isn't always simple or practical.

Table 1
Summary of XAI methods.

Type	Method	Applicable ML Models	Reference
Feature-based methods	SHAP	Linear and non-linear models	(Lundberg and Lee, 2017)
	SAGE	Linear and non-linear models	(Covert et al., 2020)
	CAM	CNN	(Zhou et al., 2016)
	Grad-CAM	CNN	(Selvaraju et al., 2020)
	DeepLIFT	DNN	(Shrikumar et al., 2017)
Global methods	Saliency maps	NN	(Simonyan et al., 2013)
	GAM	NN	(Ibrahim et al., 2019)
	DAM	NN	(Ancona et al., 2017)
Surrogate methods	LIME	Linear and non-linear models	(Dieber and Kirrane, 2020)
Pixel-based methods	LRP	NN	(Bach et al., 2015)
Concept-based method	CAV	NN	(Kim et al., 2017)

SHAP = SHapley Additive exPlanation, SAGE = Shapley Additive Global importance, CAM = Class Activation Maps, Grad-CAM = Gradient-weighted Class Activation Mapping, DeepLIFT = Deep Learning Important FeaTures, GAM = Global Attribution Mapping, DAM = Deep Attribute Map, LIME = Local Interpretable Model-agnostic Explanations, LRP = Layer-wise Relevance Propagation, CAV = Concept Activation Vectors, NN = Neural Network, DNN = Deep Neural Network, CNN = Convolutional Neural Network.

3.1.2. SAGE

SAGE (Shapley Additive Global importance) is a valuable XAI method that determines feature importance by measuring the predictive power of each feature (Covert et al., 2020). Unlike SHAP, which focuses on local interpretability, SAGE evaluates the overall impact of individual features in a global context. SAGE is more efficient than SHAP for complex computations because it avoids explaining single instances. However, in certain applications, such as spectroscopic analyses, explaining individual cases can be important, making SHAP a better choice in those situations.

3.1.3. CAM

A Class Activation Map (CAM) highlights areas in an image that significantly influence a CNN decision (Zhou et al., 2016). CAM identifies these influential regions by applying a weighted sum to the visual patterns detected across different spatial points within the image. In particular, a global average pooling operation is performed on the last convolutional feature map within the network, immediately preceding the output layer. The resulting pooled feature map then serves as input to a fully connected layer, where a loss function generates the final output. CAM generates a heatmap by mapping the weights from the output layer back onto the final convolutional layer, highlighting the specific areas of the input image that are most important to the CNN's classification. However, CAM requires a fully convolutional architecture and cannot be applied to pre-trained models that lack this structure. Additionally, the fully connected layer and any scaling adjustments in the map may cause some spatial information to be lost.

3.1.4. Grad-CAM

The Gradient-weighted Class Activation Mapping (Grad-CAM) technique provides visual explanations for decisions made by various CNN-based models (Selvaraju et al., 2020). Grad-CAM adapts the CAM approach to any CNN architecture without needing retraining. It processes the gradients from any target class through the final convolutional layer to calculate an importance score based on these gradients. Grad-CAM creates a localization map that shows which areas of the input image were crucial for the CNN's decisions. This technique highlights key neurons and links them with their names to give textual explanations of the model's decisions. However, Grad-CAM offers only coarse visualizations and struggles to explain images containing multiple instances of the same object.

3.1.5. DeepLIFT

DeepLIFT (Deep Learning Important FeaTures) is a technique that breaks down the output prediction of a neural network for a given input by tracing the contributions of all neurons in the network back to each input feature (Shrikumar et al., 2017). It evaluates the activation of each neuron against a 'reference activation' and assigns contribution scores based on the differences observed. DeepLIFT can distinguish between positive and negative contributions, uncovering dependencies that other methods might overlook. This method can calculate scores efficiently in a single backward pass. Unlike most gradient-based techniques, DeepLIFT uses a difference-from-reference approach. This approach allows it to convey important signals even when gradients are zero, avoiding issues that arise from discontinuities in gradients.

3.2. Global methods

3.2.1. Saliency maps

Gradient-based saliency maps are a visualization tool (Simonyan et al., 2013). This tool renders the absolute values of gradients related to input features of the most likely predicted class as a normalized heatmap. This heatmap highlights the most activated pixels, pointing out the most influential areas for the model's decisions. The technique allows users to see which features of the image are crucial in the classification. However, using the absolute value can suppress the gradients of neurons that receive negative inputs during the propagation through nonlinear layers. Like other feature-oriented methods, gradient-based saliency maps primarily serve as a tool for model diagnostics and offer limited insight into the decision-making process beyond that context.

3.2.2. GAM

Global Attribution Mapping (GAM) is used to explain the predictions of a neural network on a global scale (Ibrahim et al., 2019). GAM achieves this by treating attributions as weighted conjoined rankings of features with clear semantic definitions. One key advantage is the ability to adjust the level of detail through a tunable granularity parameter, allowing for tailored analysis of diverse subpopulations. GAM employs a pairwise rank distance matrix to compare features and uses a K-medoids clustering algorithm to group similar local feature importances into clusters. The medoid of each cluster represents the main pattern within that cluster, summarizing it as a global attribution. This method is particularly useful for exploring features among various subpopulations of samples.

3.2.3. DAM

The Deep Attribute Map (DAM) is introduced as a technique to enhance the explainability of gradient-based methods (Ancona et al., 2017). This framework compares different saliency-based explanation models, simplifying their concepts. Essentially, it involves multiplying the gradient of the output by the corresponding input to create a heatmap that explains a model's prediction. However, these explanations can be affected by noisy gradients and changes in the input. It's important to note that DAM alone fails to clarify the similarity or difference in results generated by two models.

3.3. Surrogate methods

3.3.1. LIME

Local Interpretable Model-Agnostic Explanations (LIME) is a versatile technique that explains locally optimized ML models, regardless of their type (Dieber and Kirrane, 2020). It operates by training a simpler, interpretable surrogate model that approximates the behavior of a more complex "black box" model within a localized input area. This is achieved by modifying understandable elements of the input data, such as components of an image, text elements, or fields in a dataset, and studying how these modifications influence the predictions to determine which features significantly impact the decision-making process. LIME includes tools specifically designed for image classification, text analysis, and tabular data, which help identify how features are weighted in classification decisions. However, the effectiveness and clarity of these explanations can be compromised if the parameters controlling the input modifications are chosen based on simple heuristics rather than careful analysis, potentially leading to less reliable or insightful explanations.

3.4. Pixel-based methods

3.4.1. LRP

Layer-wise relevance propagation (LRP) assigns specific rules to trace how inputs affect a multilayered neural network's output (Bach et al., 2015). This method produces a heatmap to show the pixels influencing the model's prediction and their impact level. LRP highlights pixels that positively impact the network's decision-making process. It applies to networks after training, serving as a post hoc technique. This approach simplifies the understanding of feature contributions to decisions and requires the network to use backpropagation.

3.5. Concept-based methods

3.5.1. CAV

Concept activation vector (CAV) is a technique that globally explains a neural network's internal states (Kim et al., 2017). CAVs map features understandable by humans to the network's high-level latent features. CAVs show how much these abstract features align with human-chosen concepts. Although this introduces some human bias, it allows for identifying flaws in the model's decision-making process. For example, it can reveal if the model incorrectly regards certain characteristics as important.

4. Application in quality assessment of agri-food products

XAI has emerged as a pivotal innovation in fast, nondestructive, and high-throughput quality assessment of agricultural products using spectroscopic techniques. It enhances transparency and trust in agricultural quality assessment, addressing the black-box nature of conventional ML models with thousands of variables. XAI helps by explaining the relations between multivariable and target properties of the sample, identifying important predictive variables, and providing clear insights, which build trust. Such model explanation ensures the reliability of analysis and fosters the research and commercialization of relevant technology towards ensuring sustainable agricultural practices. Nevertheless, the increasing number of annual publications (Fig. 5) in this field highlights the growing significance of XAI for agricultural quality assessment.

Although various approaches exist for integrating XAI into spectroscopic models, most spectroscopic models reported for agricultural quality assessment rely on the post-hoc interpretability methods. These methods necessitate the development of the spectroscopic model before applying XAI for interpretation. The overall workflow of a post-hoc XAI approach, encompassing spectroscopic model development and subsequent explanation, is illustrated in Fig. 6. The process begins with sensing samples, employing techniques such as NIR spectroscopy or HSI for spectral data, followed by reference analysis for establishing ground-truth values. Spectral pre-processing methods are often applied to eliminate noise and correct baseline variations, followed by feature selection to identify the most predictive wavelengths. Predictive models are then developed using ML algorithms, including PLSR, SVM, and advanced tree-based models such as RF or CatBoost. Post-hoc XAI techniques, such as SHAP and LIME, are subsequently employed to interpret model predictions by identifying influential wavelengths and quantifying their contributions to the model's outputs.

Recently, several studies reported the application of XAI for a wide range of agricultural samples for a range of properties, including composition analysis of agri-food products, nutrient analysis of fertilizers, plant disease detection, and biomass analysis. The application of XAI for agricultural quality assessment is summarized in Table 2.

Grapes are the cornerstone of the wine industry, where grape quality indexes directly influence the flavor, aroma, and overall quality of wine,

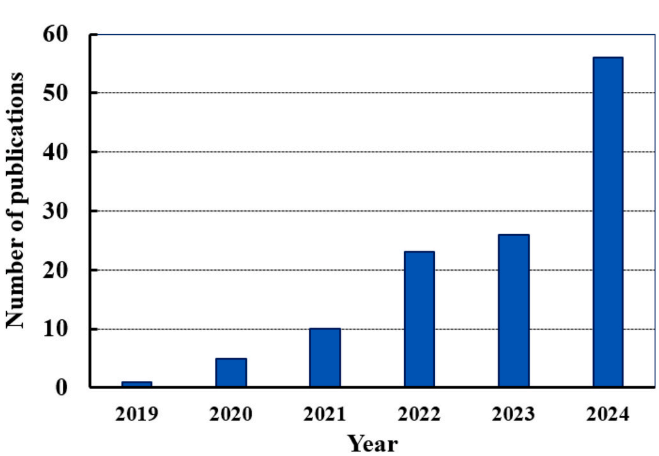

Fig. 5. Search result of "explainable AI in agriculture" in Scopus database (Elsevier, 2024).

shaping the wine market value and consumer satisfaction. A novel approach using spectroscopy and XAI has recently been reported for fast and nondestructive prediction of wine grape quality attributes. Kolasepa et al. (2023a) developed PLSR, RF, SVR, and CNN models for predicting pH, titratable acidity, and Brix content to assess the maturity index for wide varieties (e.g., Chardonnay, Malagouzia, Sauvignon Blanc, and Syrah) of wine grapes. They proposed a multi-input–multi-output CNN model with $R_p^2 > 0.80$ for almost all quality parameters across all varieties. However, they used a multi-head attention mechanism for model explanation. They highlighted that their proposed multi-input–multi-output model focused on spectral regions associated with the presence of sugars (i.e., glucose and fructose) and of the carboxylic acid group. In another study, Kolasepa et al. (2023b) used the same varieties of grapes to develop prediction models for sugar content in wine grapes. They used multiple variable selection techniques for developing robust PLSR, RF, SVR, and CNN models. Finally, they used Shapley additive global importance and Gini score plots for model explanation and identified the critical wavelengths for the sugar content of grapes. Such model explainability would help identify the critical chemical markers and spectral regions most relevant to grape maturity, enabling more targeted and efficient spectroscopic analysis while enhancing the interpretability and reliability of predictions in the wine industry.

Corn kernels play a vital role in the agricultural and food processing industries, where rapid and accurate analysis of their quality parameters is critical for optimizing production and ensuring product consistency. Spectroscopy combined with XAI techniques was reported as a reliable approach for assessing key attributes like moisture, protein, fat, and starch content. Ahmed and Kamruzzaman (2024) used NIR spectroscopy with several variable selection techniques and SHAP XAI to enhance the prediction of corn quality attributes (moisture, fat, protein, and starch). They selected multiple important wavelengths related to each quality attribute and developed a PLSR model with perfect prediction ($R^2p = 1$). Finally, the SHAP plot reveals the importance of the selected wavelengths, highlighting that XAI could facilitate the industrial application of NIR spectroscopy and lead to the development of cost-effective, real-time spectroscopic devices. Runyu Zheng et al. (2024) used 120 corn samples from seven countries for moisture and protein prediction by spectroscopic and XAI techniques. They applied chemometric methods, including PLSR model development, gradient boosting machines (GBMs) such as CatBoost and LightGBM for feature selection, and SHAP for model interpretation. Even though CatBoost Light GBM identified some effective wavelengths related to moisture (1409, 1900, 1908, 1932, 1953, 2174 nm) and protein (887, 1212, 1705, 1891, 2097, 2456 nm) prediction of corn kernel while SHAP plots further highlighted that 2174 nm and 1891 nm has the maximum contribution to the moisture and protein model respectively.

The quality assessment of sweet potatoes is crucial in postharvest management, as it directly influences consumer satisfaction, nutritional content, and market competitiveness. Ahmed et al. (2024a) used spectral data from three sweet potato varieties (e.g., Bayou Belle, Murasaki, and Orleans) from the HSI technique for developing PLSR prediction models for dry matter content (DMC), soluble solid content (SSC), and firmness. They proposed a robust PLSR model with only 7 wavelengths for each parameter using genetic algorithm (GA) and competitive adaptive reweighted sampling (CARS) methods. The best PLSR models achieved $R^2p = 0.92$ for DMC (using GA features), R^2=0.66 for SSC (using CARS features), and R^2p=0.85 for firmness (Using CARS features). The significance of the selected features in the best-performing model for each parameter was analyzed using SHAP bar and beeswarm plots, as presented in Fig. 7**.** The bar plots show feature importance based on mean absolute SHAP values, while the beeswarm plots highlight the impact and correlation of specific wavelengths on the quality prediction. Features are ranked vertically by importance, with broader SHAP value ranges indicating greater relevance to the model's predictions. The Fig. 7**a** highlights the most influential wavelengths for

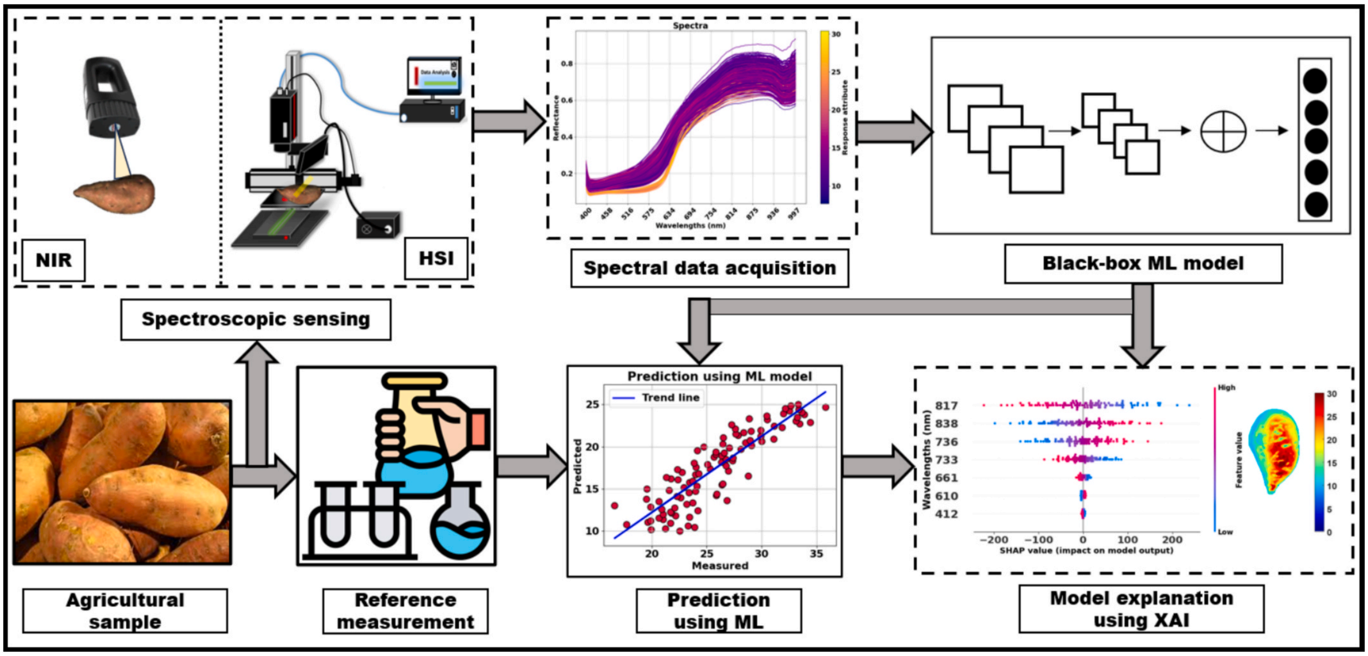

Fig. 6. Overall process flow of using XAI for a spectroscopic model for quality analysis of an agricultural product.

DMC prediction, particularly 817 nm, followed by 838, 736, and 733 nm, all from the NIR region, which align with the third overtone of O–H bonds linked to moisture drying in DMC calculation. Similarly, Fig. 7**c** identifies 808 and 838 nm as critical wavelengths for firmness prediction, while Fig. 7**b** shows that wavelengths in the 550–680 nm range, particularly 551 nm, are most important for SSC prediction in sweet potatoes. This model explanation provides valuable insights into the contribution and significance of specific wavelengths, enabling a deeper understanding of the predictive mechanisms and supporting the development of more accurate and interpretable models for sweet potato analysis.

Ageh et al. (2024) utilized various machine learning techniques, including MLR, RF, KNN, DT, and GB, combined with SHAP XAI for feature importance analysis to predict head rice yield (HRY), brown rice yield (BRY), and milled rice yield (MRY) in glutinous rice. The model achieved excellent predictive performance with R_p^2=0.99 for HRY. The SHAP beeswarm plots show that drying temperature is the most influential factor for HRY prediction, while storage temperature significantly impacts BRY and MRY predictions. Storage time and drying temperature also contribute but with lesser influence, highlighting the distinct effects of these features on rice yield quality. Zhang and Abdulla (2023) developed two CNN models and applied five normalization techniques to differentiate honey from 23 botanical sources. Integrating 11 XAI algorithms, including Saliency, Grad-CAM, DeepLIFT, SHAP, and Perturbation, with the CNN, they created an advanced wavelength selection method for honey analysis. Experimental results showed that the CNN achieved a macro average F1 score of $\geq$ 0.99 using only 8 spectral bands selected based on averaged XAI feature importance scores, establishing a methodological foundation for a cost-effective multispectral imaging system to identify honey's botanical origin.

Fast and non-destructive plant disease detection using optical sensing techniques like spectroscopy and HSI enables early identification of diseases, preserving plant health while minimizing crop losses. Nagasubramanian et al. (2019) used a 3D deep convolutional neural network (3D CNN) to effectively learn disease-specific features for detecting charcoal rot disease in soybean stems using the HSI technique. The 3D DCNN achieved a classification accuracy of 95.73 % and an F1 score of 0.87 for identifying infected samples, demonstrating its effectiveness in distinguishing between healthy and diseased plant tissues. As an XAI technique, saliency maps highlighted key pixel locations and spectral bands, revealing the model's focus on visible disease symptoms and the NIR range for accurate detection. Recently, Nguyen et al. (2024) explored the application of HSI combined with various machine learning algorithms, including tree-based methods, distribution-based approaches, geometric models, neural networks, and ensemble learning techniques to detect early-stage fungal infections in bok choy (Brassica rapa subsp. chinensis). Among these, the Multi-Layer Perceptron (MLP) neural network demonstrated superior performance, achieving an overall accuracy of 95.9 % $\pm$ 0.26 %. The MLP models could differentiate between healthy and infected plants with 99 % precision after one day of infection and distinguish between infections caused by F. commune and R. solani with 99 % precision after two days, notably before any visible symptoms appeared. The researchers used the SHAP explainable AI technique to interpret the MLP models, identifying key spectral regions (445–460 nm, 560–595 nm, 606–620 nm, and 719–728 nm) strongly associated with fungal infections in bok choy.

Determining macronutrients in fertilizers and plant biomass is crucial for optimizing plant growth, diagnosing nutrient deficiencies, and improving crop yields by guiding effective agricultural practices. Nondestructive macronutrient analysis by green tools like spectroscopy and HSI supports sustainable resource management by evaluating biomass quality for energy, feedstock, and soil health while minimizing environmental impacts. Guindo et al. (2023) assessed laser-induced breakdown spectroscopy (LIBS) and Vis-NIR spectroscopy sensors for rapid detection of phosphorus (P) and potassium (K) in organic fertilizers. SHAP values were utilized to identify significant variables from both types of sensor data. Then, the characteristic variables from both spectroscopic sensors were combined to form the spectra fusion. The SVR, PLSR, and Extremely Randomized Trees (ExtraTrees) models showed that XAI-based fusion outperformed single-sensor approaches, achieving R2 values of 0.9946 for P and 0.9976 for K, with significantly lower RMSE and higher RPD. Dehghan-Shoar et al. (2023) reported a hybrid model that integrates empirical and physically based approaches to estimate nitrogen concentration (N%) using a large grassland data set (>6000 samples) grown in diverse environments in New Zealand. The hybrid model achieved an RMSE of 0.27 % N, an R2 of 0.78, and a mean prediction interval width of 0.26, outperforming both standalone empirical and physically based models. SHAP values identified key

Table 2
Application of XAI for spectroscopic analysis of agricultural products.

Sample type	Quality attribute	Spectral range (nm)	Spectral model	XAI method used	XAI application reason	Analytical results	Reference
Grape	SSC, pH, and TA	350–2500	PLSR, RF, SVR, CNN	Multi head attention	Feature importance	$R^2 = 0.79$ (using CNN)	(Kalopesa et al., 2023b)
	SSC	350–2500	PLSR, RF, SVR, CNN	SAGE	Feature importance	$R^2 = 0.82$ (SSC) $R^2 = 0.76$ (pH) $R^2 = 0.79$ (TA)	(Kalopesa et al., 2023a)
Corn kernel	Moisture, Protein, Fat, Starch	1100–2498	PLSR	SHAP	Feature importance	$R^2p = 1.00$	(Ahmed and Kamruzzaman, 2024)
	Moisture, Protein	867–2535	PLSR	SHAP	Feature importance	$R^2p = 0.97$ (Moisture)	(Zheng et al., 2024)
Sweet potato	DMC, SSC, Firmness	400–1000	PLSR	SHAP	Feature importance	$R^2p = 0.92$ (DMC)	(Ahmed et al., 2024a)
	DMC	400–1000	PLSR	SHAP	Feature importance	$R^2p = 0.88$ (using reconstructed spectra)	(Ahmed et al., 2024b)
	Firmness	400–1000	CNN	SHAP	Feature importance	Rp = 0.84	(Ahmed et al., 2025d)
Glutinous rice	HRY, BRY, MRY	450–998	MLR, RF, KNN, DT, GB	SHAP	Feature importance	$R^2 = 0.99$ (HRY)	(Ageh et al., 2024)
Honey	Thickness	399–1064	CNN	Saliency, Grad-CAM, DeepLIFT, SHAP	Feature selection	F-1 score = 99.06 %	(Zhang and Abdulla, 2023)
Soybean stem	Charcoal rot infection	350–2500	3D-CNN	Saliency map	Visualization	Accuracy = 95.73 %	(Nagasubramanian et al., 2019)
Bok choy	Disease detection	400–1000	RF, XGB, LR, QDA, GP, SVM, MLP, TabNet, LSTM	SHAP	Feature importance	Accuracy = 95.90 % (using MLP)	(Nguyen et al., 2024)
Organic fertilizers	Macronutrients	229–1000	SVR, PLSR, Extratrees	SHAP	Feature importance	$R^2p = 0.99$	(Guindo et al., 2023)
Grassland	Nitrogen	350–2500	GPR	SHAP	Feature importance	$R^2 = 0.78$	(Dehghan-Shoar et al., 2023)
Solid waste	Carbon content	935–1720	RF, XGB, LGBM	SHAP	Feature importance	Accuracy = 98.10 %, $R^2 = 0.98$	(Lan et al., 2023)
Eggs	Gender	383–1011	ViT	Grad-CAM, SHAP	Feature importance	Accuracy = 95.40 %	(Ji et al., 2024)
	Fertility	374–1015	XGBoost, CatBoost, RF, SVM	SHAP	Feature importance	Accuracy= 95.1 %	(Ahmed et al., 2025b)
	Shell thickness	1300–2525	PLSR	SHAP	Feature importance	$R^2p = 0.91$	(Ahmed et al., 2025c)

SSC= Soluble Solid Content, TA = Titratable Acidity, CNN = Convolutional Neural Network, RF = Random Forest, SVM = Support Vector Machine, SVR = Support Vector Regression, PLSR = Partial Least Squares Regression, XGB = Extreme Gradient Boost, LGBM = Light Gradient Boost, SAGE = Shapley Additive Global importance, Extratrees = Extremely Randomized Trees, GPR = Gaussian Process Regression, DMC = Dry matter content, MLR = Multiple Linear Regression, KNN = K-Nearest Neighbors, DT = Decision Trees, GB = Gradient Boosting, HRY = Head Rice Yield, BRY = Broken Rice Yield, MRY = Milled Rice Yield, ViT = Vision Transformer.

spectral features, notably 2052 nm and 852.5 nm, as significantly influencing nitrogen concentration predictions, explaining their critical role in driving the model's output. Lan et al. (2023) determined the proportions of biogenic and fossil carbon in solid waste using HSI and XAI. They developed random forest, XGBoost, and light GBM models for carbon prediction and SHAP explainable AI for model explanation. All classifiers and regressor models achieved an accuracy above 0.95 and an R2 of 0.96 on the validation set. The SHAP analysis emphasized the significance of overtones and combinations of the C–H, N–H, and O–H functional groups. Notably, the C–H functional group emerged as the most critical factor influencing the prediction of carbon content in solid waste.

Nondestructive identification of egg sex during incubation is essential for improving animal welfare and reducing the culling of male chicks in poultry production. Recently, several nondestructive optical sensing techniques were reported for egg sex classification. Even though some studies reported promising prediction results of different black box prediction models, for the commercialization of technology, it is crucial to understand the significant variables related to egg sex. Recently, Ji et al. (2024) reported HSI-based EggFormer model for egg sex prediction during early incubation leveraging channel attention and transformer self-attention mechanisms. RF, PCA, SPA, and CARS algorithms were used to select important variables for robust model development. Consequently, GRAD-Cam and SHAP explainable AI is used to explain the best prediction model. The EggFormer model demonstrated superior results, with an accuracy of 95.4 %, recall of 98.6 %, F1 score of 0.958, and Kappa of 0.908. The XAI analysis reveals that wavelengths in the 700–800 nm range are critical for the model's performance, with the most influential wavelengths being 712.76 nm, 765.33 nm, 722.97 nm, 714.22 nm, and 695.3 nm, as indicated by higher SHAP values.

5. Limitations, opportunities, and future directions

XAI acts as a critical bridge between machine intelligence and domain expert understanding. It aims to increase the acceptance of AI systems by making them interpretable to specialists in their respective fields. Real-world applications of XAI present significant opportunities to enhance model interpretability, stakeholder trust, and decision-making transparency. Specifically, applications in finance, where XAI techniques have been used to explain credit card default predictions (De et al., 2020), forecasting, where semantic and AI technologies were deployed for demand forecasting while ensuring confidentiality (Rožanec et al., 2022), and healthcare, where methods like SHAP and Grad-CAM have improved trust and interpretability in disease prediction, including myocardial infarction detection, skin cancer classification, and Alzheimer's disease prediction (Saranya and Subhashini, 2023). Additionally, in remote sensing, XAI has improved classification tasks through deep learning (Kakogeorgiou and Karantzalos, 2021). It has also been applied in signal processing, where CNN-based XAI methods have been used for vibration signal analysis (Kim and Lee,

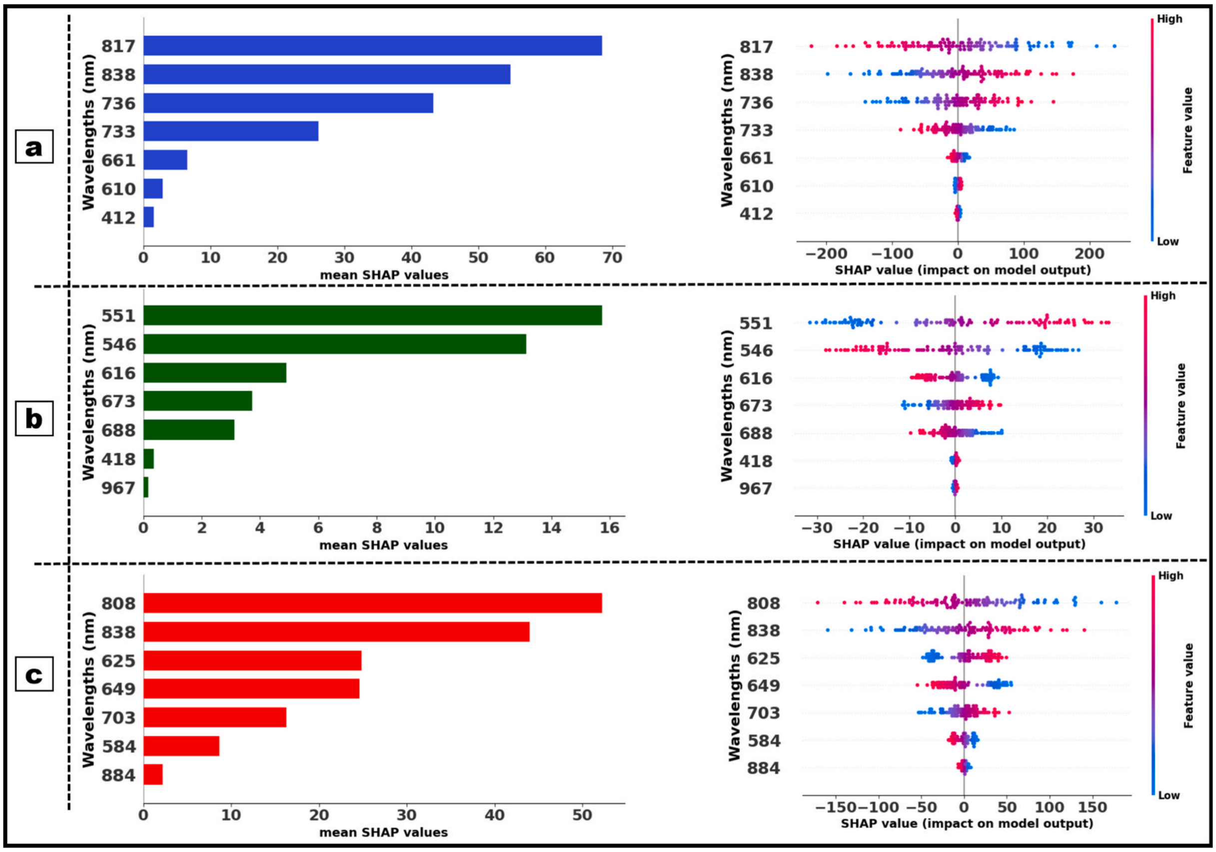

Fig. 7. SHAP feature importance bar (left) and beeswarm (right) plots for the prediction of (a) DMC (%), (b) SSC (Brix), and (c) Firmness (N) content of sweet potato using VNIR-HSI spectra (Ahmed et al., 2024a).

2022). Inspired by its applications in established domains, XAI holds the potential to enhance transparency and trust in the less-explored field of agricultural spectroscopy. Spectral data often include hundreds of collinear wavebands, making it difficult to interpret meaningful patterns from these high-dimensional details (Kamruzzaman et al., 2022). Additionally, spectroscopic data are sensitive to environmental and instrumental conditions, meaning even small changes in the experimental setup can affect model explainability. While spectral AI systems provide significant advantages, there are concerns about granting them extensive decision-making authority without adequate transparency. This transparency is vital for understanding AI decisions and for fostering the development of more human-centric spectroscopic solutions. Since the design of most spectroscopic systems is highly domain-specific, even minor changes in spectral analysis, such as feature selection or contribution, can have significant impacts.

Additional limitations in the field of XAI on spectral models for agricultural product quality evaluation merit further examination. One significant issue is the tradeoff between model explainability and performance. It has been observed that complex spectral models often outperform simpler, more transparent ones. This tradeoff frequently compels researchers to prioritize performance enhancements at the expense of explainability. Nevertheless, several studies have challenged this tradeoff by demonstrating that well-explained spectral models can achieve comparable performance (Dziugaite et al., 2020; Wang et al., 2017). Moreover, the evaluation metrics for XAI methods are seldom explored within the agricultural sector. These metrics are crucial for assessing a model's effectiveness. In XAI contexts, they provide comprehensive assessments of how well a model adheres to XAI standards, including measures of explanation satisfaction, explanation quality, and scale validations such as discriminant and content validity (Minh et al., 2022). XAI metrics encompass both quantitative and qualitative indicators, essential for thorough evaluations. Therefore, it is essential to assess these metrics in spectral analyses to ensure the robustness and reliability of the models. Additionally, interpreting results from complex models like deep learning can be very difficult. These models often operate in high-dimensional spaces with non-linear functions, making them more complex than simpler, low-dimensional models. Besides, deep learning models can strain embedded or mobile devices due to the high number of calculations and memory access required. This makes it challenging to integrate explainable deep learning with resource-limited platforms (Chen et al., 2020). Current methods used to explain these deep learning models can easily be misled by simple tricks. Research has shown that neglecting bias terms and altering input data during pre-processing can deceive these networks (Kindermans et al., 2019; Wang et al., 2019). Since pre-processing is a typical step in analyzing data, it's not wise to fully trust the outputs from a highly accurate spectral model without proper explanation. Besides, deep and machine learning models are susceptible to adversarial attacks that deliberately manipulate input data to degrade model performance. These attacks introduce subtle noise into data like images, videos, audio, and text. The changes are often undetectable to the human eye, especially in agricultural images (Alferidah and Algosaibi, 2024). XAI models can help by improving trust in these models by increasing interpretability. They also strengthen security and make agricultural models more resistant to such attacks (Tasneem and Islam, 2024).

Despite their limitations, XAI techniques can greatly benefit the agricultural sector when used in spectral analyses. XAI enhances the clarity of feature selection in spectral models, which is crucial for industrial applications. Understanding the importance of specific features in a spectral model adds significant value. Additionally, XAI methods can be adapted to meet the needs of spectral analysis applications. With the improvement of domain-specific AI models, such as physicsinformed machine learning, XAI techniques can be modified for clearer explanations of these models. Moreover, XAI is crucial for complying with regulations that demand trustworthy modeling, especially in sensitive areas like food safety. Although spectral analyses are sensitive to environmental conditions, robust XAI models can be extremely beneficial. Besides, XAI can significantly advance the development of innovative computational spectral analysis techniques. For example, XAI can enhance transparency in deep learning-based HSI reconstruction methods (Ahmed et al., 2025e, 2024c, 2024d). Besides, XAI requires no additional hardware beyond what is needed to train these spectral deep-learning models (Höhn and Faradouris, 2021). However, integrating XAI into spectroscopic analyses presents challenges, which act as a bottleneck for its broader application across various fields. Developing user-friendly, interactive spectroscopic XAI tools could facilitate interdisciplinary research and maximize the benefits of this emerging technology (Ahmed et al., 2024e). In conclusion, XAI techniques are poised to become a crucial tool for increasing trust and understanding of complex spectroscopic models, thereby improving operational efficiency.

6. Conclusions

The advent of deep learning has made spectroscopic models more accurate and practically applicable in agriculture. However, users often lack a clear understanding of these models' internal mechanisms and the contribution of individual features. This lack of transparency can limit the application and innovation of agricultural spectroscopic analyses, where selecting the appropriate spectral wavelengths is critical. Integrating XAI techniques is therefore essential in this field. This systematic review emphasizes the transformative potential of XAI in fostering trust and transparency in agricultural practices, food quality assessment, and postharvest evaluation. As the technologies continue to evolve, XAI methods are expected to enable more advanced, precise, and extensive spectroscopic applications. This progress has the potential to revolutionize agriculture and food engineering, unlocking new research opportunities and improving operational efficiency.

CRediT authorship contribution statement

Md.Toukir Ahmed: Writing – review & editing, Writing – original draft, Methodology, Investigation, Conceptualization. **Md Wadud Ahmed:** Writing – review & editing, Writing – original draft, Methodology. **Mohammed Kamruzzaman:** Writing – review & editing, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgment

This work was funded by the U.S. Department of Agriculture Agricultural Marketing Service through the Specialty Crop Multistate Program grant AM21SCMPMS1010. The contents are solely the responsibility of the authors and do not necessarily represent the official views of the USDA.

Data availability

No data was used for the research described in the article.

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