



Rapid Detection and Quantification of Adulterants in Turmeric Using Fourier Transform Infrared (FTIR) Spectroscopy Coupled with Advanced Statistical Models

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Abstract

Turmeric, valued for its culinary and medicinal properties, has increasingly become vulnerable to harmful adulteration, posing serious health risks. Among these, ferrous sulfate heptahydrate is particularly concerning due to its potential to cause iron overload and oxidative stress. This study intended to develop a rapid, cost-effective, and non-destructive technique for finding such adulteration using Fourier Transform Infrared (FTIR) spectroscopy in Attenuated Total Reflectance (ATR) mode. Fresh turmeric samples collected from five locations in Tamil Nadu, India, were mixed with ferrous sulfate heptahydrate at concentrations of 0%, 5%, 10%, 15%, 20%, 25%, 30%, and 100%, yielding a total of 36 samples. FTIR spectra revealed distinct peaks for turmeric (1630 cm^{-1} , 1745 cm^{-1} , 2930 cm^{-1} , 3720 cm^{-1}) and for the adulterant (1060 cm^{-1}), providing clear spectral markers for adulteration detection. The spectral dataset was analyzed using Multiple linear regression (MLR), random forest (RF), K-nearest neighbors (KNN), eXtreme Gradient Boosting (XGBoost), and Artificial neural networks (ANN). Among these, XGBoost achieved the peak overall performance, through an R^2 of 0.9968, mean squared error (MSE) of 0.0007, root mean squared error (RMSE) of 0.0265 (dimensionless), and very low mean absolute error (MAE). ANN also produced comparable accuracy, confirming the robustness of nonlinear approaches. These findings demonstrate that combining FTIR with advanced machine learning, particularly XGBoost, provides a powerful framework for rapid, reliable, and non-destructive adulteration detection in turmeric, with potential applicability to other food powders.

Keywords eXtreme gradient boosting · Artificial neural network · Multiple linear regression · FTIR spectroscopy · Adulteration · K-nearest neighbors

Abbreviations

Nomenclature

β_0	Coefficients of MLR
l_m	Impurity
k	Nearest neighbors
$L_{(\varphi)}$	Regularization function

Ω	Minimum loss
Y	Branch weight

Abbreviations

MLR	Multiple linear regression
ANN	Artificial neural networks
PCM	Phase change material
ISD	Indirect solar dryer
TSM	Thermal storage material
RMSE	root mean squared error
NIR	Near-infrared
FTIR	Fourier Transform Infrared
ATR	Attenuated Total Reflectance
PLS	Partial Least Squares
RF	Random Forest
KNN	K-nearest neighbours
MSE	mean squared error
MAE	mean absolute error

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PCR Principal Component Regression
LDA Linear Discriminant Analysis

Introduction

Turmeric (*Curcuma longa* L.) is among the greatest widely cultivated spices in India, which contributes near 80% of the global supply. Annual production exceeds 400,000 tons, harvested from an estimated 50,000 acres of farmland, positioning the country as the leading producer and exporter of turmeric (Dhakal et al. 2019). Owing to its distinctive color, flavor, and bioactive compounds, turmeric has found applications far beyond its culinary role. The rhizome is rich in curcuminoids, which impart a golden-yellow hue and are responsible for a varied range of biological activities. These contain antioxidant, anti-inflammatory, and antimicrobial properties that support its use in traditional medicine as well as modern pharmacological formulations (Cousins et al. 2007; Dhiman et al. 2024; Kalluru et al. 2020). Turmeric's widespread adoption in food, medicine, and textile industries underscores its economic and health significance. The rising global demand for turmeric has, however, made it highly vulnerable to adulteration. Substances such as chalk powder, lead chromate, and synthetic dyes have been historically used to increase bulk or intensify color (Bansal et al. 2017). More recently, ferrous sulfate heptahydrate has been identified as a serious adulterant. While it may visually resemble turmeric due to its yellowish tint, its consumption can cause iron overload, oxidative stress, and gastrointestinal distress, and long-term exposure may contribute to chronic conditions such as liver damage and cardiovascular disorders (Vignesh et al. 2025). Reported incidents of turmeric contamination with metallic salts highlight the public health risks posed by such practices, reinforcing the need for robust detection strategies. Conventional detection methods, including microscopic inspection, spot tests, and chromatographic methods, have been employed to identify adulterants in turmeric. These approaches, however, suffer from key drawbacks. Microscopy requires expert interpretation and is not suited for large-scale screening. Chemical assays are often destructive, qualitative, and limited in sensitivity. Chromatographic methods, while accurate, involve costly instrumentation and lengthy preparation steps. Together, these limitations hinder the feasibility of routine monitoring in supply chains. In response, spectroscopic techniques have gained attention for their ability to deliver rapid, non-destructive, and environmentally friendly scrutiny of powdered foods and spices (Mei et al. 2022). Near-infrared (NIR) spectroscopy, which probes molecular bonds in the 780–2526 nm region, has been widely used to assess food composition, while visible (VIS) spectroscopy captures information in the 380–780 nm range and is closely linked to color characteristics (Zhang

et al. 2023). Fourier Transform Infrared (FTIR) spectroscopy has emerged as a particularly effective tool due to its ability to generate molecular fingerprints with minimal sample preparation, high reproducibility, and real-time capability (Contla Hernández et al. 2021). Nevertheless, FTIR spectra often exhibit broad and overlapping absorption bands, which make manual interpretation challenging (Huang et al. 2022).

To overcome these challenges, machine learning (ML) algorithms have been increasingly applied to spectroscopic data. By capturing nonlinear and high-dimensional patterns, ML improves classification and prediction beyond the capacity of traditional statistical techniques such as Partial Least Squares (PLS), Linear Discriminant Analysis (LDA), Principal Component Regression (PCR), and multiple linear regression (MLR) (Khan et al. 2015). Recent research has successfully combined spectroscopy with ML for detecting adulteration in milk (Chu et al. 2024), herbal medicines (Chen et al. 2024), honey (Razavi and Kenari 2023), and meat (Rady et al. 2021), demonstrating the potential of these integrated approaches for food authenticity studies.

Building on these advances, the present study applies FTIR spectroscopy in Attenuated Total Reflectance (ATR) mode to detect and quantify adulteration of turmeric with ferrous sulfate heptahydrate. Multiple ML models—MLR, K-nearest neighbors (KNN), Random Forest (RF), Artificial neural networks (ANN), and eXtreme Gradient Boosting (XGBoost)—are employed to analyze spectral data and evaluate predictive performance.

The main purposes of this work are the following:

- To examine the potential of FTIR spectroscopy in ATR mode for identifying ferrous sulfate heptahydrate adulteration in turmeric, with emphasis on distinguishing its characteristic spectral bands.
- To assess and compare the performance of machine learning models—RF, MLR, KNN, ANN, and XGBoost—when applied to FTIR spectral datasets for adulteration detection.
- To select the greatest accurate and reliable model based on evaluation metrics such as R^2 , MSE, RMSE, and MAE, and propose an efficient framework for practical food quality monitoring.

Materials and Methods

Material and Sample Preparation

Fresh turmeric rhizomes were procured from local farmers across five different regions in Tamil Nadu, India, to capture variability in source material. After cleaning and rinsing, the rhizomes were briefly boiled for 2 min, a process known to reduce microbial load, decrease raw odor, gelatinize starch,

ANN Regression

The ANN regression model demonstrated strong predictive ability for adulteration levels. Its architecture consisted of three fully connected layers: an input layer with 64 neurons, a hidden layer containing 32 neurons, and a final output layer with a single neuron. After optimization, the ANN achieved an R^2 value of 0.9990, with error metrics of $MSE = 0.0020$, $RMSE = 0.045$, and $MAE = 0.012$, indicating near-perfect prediction accuracy. These results demonstrate the ANN's ability to capture the nonlinear spectral–concentration relationships inherent in the FTIR dataset, outperforming simpler regression methods. Figure 6 illustrates the training and validation loss curves over multiple epochs. Both curves decreased steadily and stabilized at low values without divergence, confirming that the model generalized well and avoided overfitting despite the relatively small dataset size. This highlights the robustness of the ANN regression approach for this application. When compared with other models, ANN, XGBoost, and KNN all achieved very high

R^2 scores (≈ 0.999) with minimal error values. While ANN demonstrated strong adaptability in capturing nonlinear interactions, XGBoost provided greater interpretability through feature importance analysis. Thus, although both models offer highly accurate predictions, the choice for practical deployment may depend on the trade-off between interpretability and computational complexity.

Conclusion

This paper work demonstrated the effectiveness of integrating FTIR spectroscopy with machine learning algorithms to detect ferrous sulfate heptahydrate adulteration in turmeric. Among the models tested, XGBoost emerged as the best-performing algorithm, achieving very high predictive accuracy ($R^2 > 0.99$) with minimal error values. The ANN model also delivered comparable accuracy, confirming the robustness of nonlinear approaches for this task.

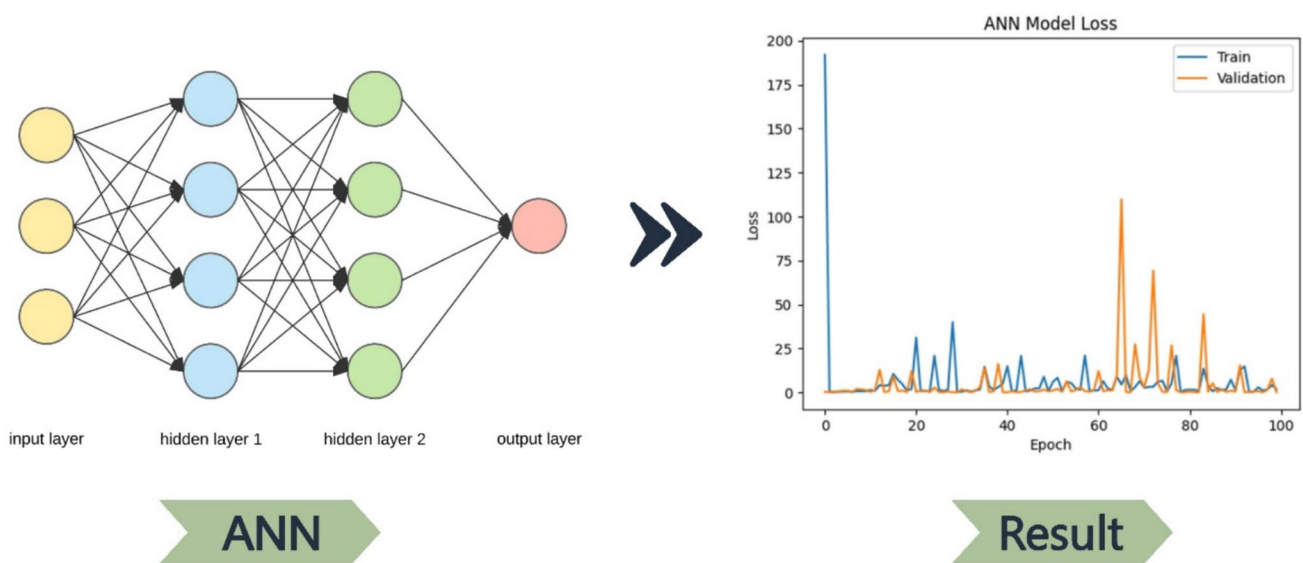


Fig. 6 Training and validation loss of the ANN model

Key conclusions are as follows:

- **High Predictive Accuracy:** XGBoost and ANN both outperformed traditional regression methods, highlighting their suitability for complex FTIR datasets.
- **Model Selection:** While ANN achieved slightly higher predictive scores, XGBoost provided greater interpretability through feature importance analysis, making it a more practical choice for real-world applications.
- **Practical Implications:** The combination of FTIR and machine learning enables rapid, reliable, and non-destructive

- **Future Scope:** Enlarging the dataset, applying cross-validation techniques, and testing additional adulterants will further improve generalizability and facilitate adoption in industry and regulatory settings.

In conclusion, FTIR spectroscopy coupled with advanced machine learning—particularly XGBoost—offers a powerful and scalable framework for ensuring the authenticity and safety of turmeric and similar powdered food products.

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Author Contributions A. formulated the work, B. Supervisor for A. and supported analysis of the samples and reviewed the work and C. Reviewed the work and provided valuable suggestions.

Data Availability The Data will be shared upon the request.

Declarations

Competing interests The authors declare no competing interests.

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