RESEARCH PAPER

Rapid forensic differentiation of soil samples using FTIR – LDA approach

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ABSTRACT

Soil is a valuable source of trace evidence in forensic investigations because it can link individuals or objects to specific areas. This study assesses a quick and non-destructive method for discriminating soil samples using Fourier-transform infrared (FTIR) spectroscopy and linear discriminant analysis (LDA). Twelve soil samples were obtained from industrial, agricultural, and riverfront sites in four districts of Andhra Pradesh, India. A Bruker Alpha spectrometer was used to obtain FTIR spectra ranging from 4000-400 cm^{-1}. A binary presence-absence matrix of transmittance peaks was created to reflect functional group occurrence. This matrix underwent direct LDA without any prior dimensionality reduction. The generated score plot demonstrated sample grouping based on sampling sites. The Smalldon and Moffat method yielded a discrimination power of 68.18%, showing moderate differentiation among soil pairs. These findings indicate that FTIR-LDA can be used as a quick preliminary tool for forensic soil discrimination, especially when paired with complementary analytical or machine learning techniques.

Keywords: Forensic, soil analysis, FTIR-LDA, machine learning, trace evidence.

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INTRODUCTION

In forensic investigations, soil is a crucial type of trace evidence that can offer critical details for connecting victims or suspects to a crime scene. Recovered dirt from clothing, shoes, car tires, and other items may still have unique physical and chemical properties that make it possible to compare it to soil from a suspected location. Forensic soil investigation has used a variety of analytical approaches, from microscopic inspection to sophisticated instrumental techniques including spectroscopy and X-ray fluorescence (XRF) [1]. Fourier-transform infrared (FTIR) spectroscopy is one of these techniques that has attracted a lot of interest since it is quick, non-destructive, and requires little sample preparation [2]. Through distinctive spectral fingerprints, FTIR makes it possible to identify both organic and inorganic components in soil. Chemometric techniques like principal component analysis (PCA) and linear discriminant analysis (LDA) are widely used for sample classification and discrimination in order to improve the interpretation of complex spectrum information [3, 4, 1]. The reliability of forensic soil comparisons is still impacted by issues such as soil composition variability, a lack of established techniques, and a lack of datasets [5], despite growing interest in FTIR-based soil analysis [4]. In this regard, the current work assesses the viability of differentiating soil samples taken from several sites in Andhra Pradesh, India, utilizing FTIR spectral peaks in conjunction with direct linear discriminant analysis [5]. In the current research, LDA was used on FTIR data, with a focus only on transmittance peaks, to determine the feasibility of such a technique. Despite growing interest in

FTIR-based soil analysis, some hurdles persist, including soil composition heterogeneity, insufficient datasets, and a lack of defined analytical procedures. These factors can have an impact on the accuracy and reproducibility of forensic soil comparisons [6]. In this respect, the current study assesses the feasibility of separating soil samples taken from several locations in Andhra Pradesh, India, utilizing FTIR-derived spectral peaks and direct linear discriminant analysis.

Methodology

Sampling

Twelve soil samples were taken during the winter season (January 2024) in four districts of Andhra Pradesh, India: Visakhapatnam, East Godavari, Tirupati, and Kurnool. Samples were collected from three types of environments: industrial regions, agricultural fields, and riverbanks. To ensure spatial representation and eliminate sampling bias, topsoil was taken at random depths of 1-10 cm across each site. The samples were placed in labelled plastic containers and delivered to the laboratory for further investigation. Prior to examination, soil samples were air-dried at room temperature to eliminate moisture and stored in a clean environment to prevent contamination.

FTIR Analysis

Fourier-transform infrared spectra were obtained using a Bruker Alpha II FTIR spectrometer in the 4000-400 cm^{-1} region. The acquired spectra were examined to find transmittance peaks that corresponded to various functional groups found in the soil samples. The functional groups were assigned using an online FTIR spectrum database [7].

Chemometric Analysis

Linear discriminant analysis (LDA) was used to assess the differentiation of soil samples based on their FTIR spectrum properties. The identified transmittance peaks were used to create a binary presence-absence matrix that represented the occurrence of functional groups in each soil sample. This matrix was used as the input dataset for LDA. The strategy reduces the data to a lower-dimensional space while optimizing the ratio of between-class variation to within-class variance, resulting in better separation of designated groups.

Discrimination Power

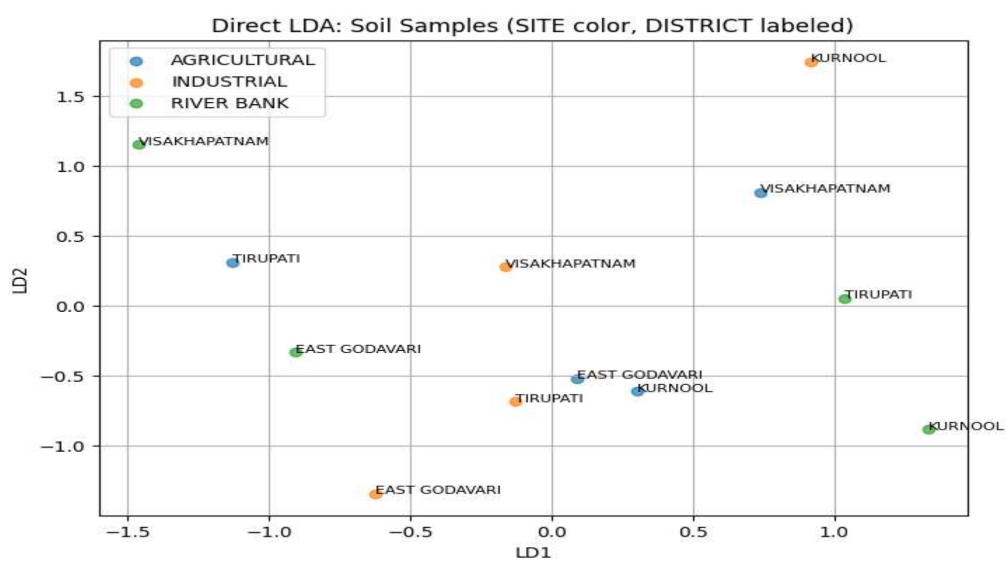
The classification method's performance was examined using Discrimination Power (DP) calculated according to the Smalldon and Moffat formula [8].

DP = Total number of discriminating pairs of samples / Total number of possible pairs of samples * 100

Total number of possible sample pairs (n) = n(n-1)/2, where n is the total number of samples.

Result

FTIR spectra in the 4000-400 cm^{-1} region showed transmittance peaks for several functional groups in soil samples. The detected peaks ranged from 3963.73 cm^{-1} to 418.07 cm^{-1}, allowing for the identification of several chemical classes. The most common functional groups were alcohols, phenols, halogenated compounds, metal-oxygen linkages, alkanes, aromatic compounds, and nitro compounds. These spectral peaks were converted into a binary presence-absence matrix that was then used for LDA analysis. The generated score map indicated sample clustering along the first two discriminant functions (LD1 and LD2). The plot shows that FTIR spectral fingerprints include enough information to distinguish soil samples from different sites. The Smalldon and Moffat formula was used to compute the discrimination power in order to quantitatively assess categorization performance. The DP value obtained in this investigation was 68.18%, indicating that the suggested approach could



correctly discriminate about two-thirds of all potential soil sample pairs.

Fig 1: Shows the LDA plot of the samples from all the districts from three region.

Discussion

The findings show that FTIR-derived spectral peaks paired with LDA can give a significant difference between soil samples taken from various geographical areas. Unlike traditional PCA-LDA procedures, the current technique uses LDA directly on a binary matrix of spectral peaks. This strategy simplifies the analytical workflow while maintaining the interpretability of the various functional groups that contribute to sample differentiation. The moderate discrimination power found in this investigation implies that FTIR spectral fingerprints alone may not always be sufficient for comprehensive forensic discrimination of soil samples. However, the procedure provides a quick and non-destructive initial screening strategy. Similar spectroscopic investigations have demonstrated that combining chemometric and spectroscopic techniques can considerably increase classification accuracy. Recent developments in spectroscopy and machine learning have yielded promising results for soil analysis. Raman spectroscopy, laser-induced breakdown spectroscopy, and visible-near infrared spectroscopy have all been effectively coupled with machine learning [9] methods like support vector machines [10], convolutional neural networks, and partial least squares regression [11]. These approaches demonstrate the value of combining advanced analytical instruments with data-driven models to improve forensic soil discrimination. Future research could improve classification performance by combining FTIR data with additional analytical techniques like X-ray spectroscopy, Raman spectroscopy [11], and chromatographic procedures [12-14]. Furthermore, combining spectral data with microscopic image analysis and powerful machine learning techniques may result in a more robust framework for forensic soil identification [15-17].

Limitations

The current model was assessed on the same dataset for both training and testing, yielding apparent classification accuracy. This study did not provide independent validation with separate training and testing datasets. Future research should use cross-validation procedures and larger datasets to increase model dependability and more accurately predict classification error.

Conclusion

This study shows that FTIR spectroscopy combined with linear discriminant analysis can be utilized to differentiate soil samples from various geographical regions in Andhra Pradesh, India. Using a binary presence-absence matrix of spectral peaks, the proposed method attained a discrimination power of 68.18%, showing

intermediate classification capacity. The findings demonstrate that FTIR spectral fingerprints can be used as a quick and non-destructive tool for preliminary forensic soil discrimination. However, because of its limited discrimination strength and the lack of defined methods in soil spectroscopy, FTIR-LDA should be combined with other analytical techniques and powerful machine-learning algorithms to improve the reliability of forensic soil comparisons.

Conflicts of interest

The authors declare no conflicts of interest.

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