Comparative Analysis of Traditional and Regularized Adaptive Deconvolution Models for Pigment Quantification in Olive Oils Using UV-Vis Spectroscopy and Machine Learning

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***Abstract*—This study takes a closer look at how well a traditional deconvolution model and a new Machine Learning (ML) approach, called the Regularized Adaptive Deconvolution (RAD) model, perform in analyzing pigment concentrations in oil samples using UV-Vis spectroscopy. Both models demonstrated excellent performance, consistently achieving R^2 values over 0.99 in reconstructing spectra for various oils. The RAD model's integration of ReLU activation functions and L2 regularization enabled it to eliminate physically impossible negative concentration estimates. Through Integrated Gradients and Saliency Maps, the model effectively captured known spectral features and highlighted subtle but important differences between oil types, providing enhanced interpretability of pigment-wavelength relationships. This reliability and the RAD model's ability to provide clearer differentiation between pigments makes it particularly valuable for real-world applications in the food industry, supporting rapid, non-destructive quality control and authenticity testing of oil products.**

***Index Terms*—Extra virgin olive oil (EVOO), UV-Vis spectroscopy, machine learning, pigment concentration, quality control**

I. Introduction

THE olive tree, scientifically known as Olea europaea L., is a plant species that originates from the Mediterranean area and has played a crucial role in the region's agriculture and culture for thousands of years. The main product obtained from this plant, olive oil, has become more popular worldwide because of its distinct sensory characteristics and multiple health advantages. Extra virgin olive oil (EVOO) is obtained straight from olives, essentially turning it into pure olive juice. It is considered the best olive oil because of its excellent features, such as acidity levels usually below 0.8% and a sensory score of over 6.5 points. These standards guarantee that EVOO has a perfect scent and taste, setting it apart from other types of olive oil [1].

EVOO is a high-quality item highly valued for its flavorful taste, health benefits, and properties that promote wellness. The pigment composition of EVOO, primarily determined by chlorophylls and carotenoids, is a crucial factor affecting its quality, color, and sensory characteristics. Chlorophylls give the oil its green color and break down the oil when exposed to light, while carotenoids add a yellow hue and provide antioxidants. The amount of these pigments affects both the visual aspect and the longevity, stability, and health benefits of the oil. Therefore, precise measurement of pigment levels is crucial for quality assurance and verifying the genuineness of EVOO [2].

The variety of carotenoids and chlorophyll derivatives found in olive oils includes β-carotene (β-CAR), lutein (LUT), violaxanthin, neoxanthin (NEX), and other xanthophylls, as well as pheophytins A (Pheo-a) and B (Pheo-b) and other minor derivatives. The original pigment composition of the olive fruits and other chemical changes, including those caused by enzymes, that take place during the stages of olive oil production affect the amount of various components in olive oil [3]. Numerous variables, including cultivar type, environment, fruit ripeness at harvest, olive sampling technique, oil production process, and storage conditions, affect the chemical composition of EVOO throughout time [4]. Since EVOO is high in heart-healthy fats and antioxidants, it is important to acknowledge it as one of the healthiest eating habits. Its consumption is associated with a number of health advantages, such as lowered risk of heart disease, decreased inflammation, and possible anti-cancer actions. These characteristics support EVOO's standing as a healthy fat in food that has major advantages for general well-being.

Conventional approaches for analyzing pigment EVOO usually entail chemical extraction, which is followed by chromatographic methods. These processes are frequently tedious, time-consuming, and need specific tools and solvents [5]. Furthermore, the content of the oil cannot be altered by simply applying these damaging processes to it. Pigment concentration analysis can be done non-destructively using spectroscopic methods, especially UV-Vis spectroscopy. UV-Vis spectrometry measures light absorbance at particular wavelengths and can provide important details about the presence and concentration of various pigments in EVOO [2]. However,

because carotenoids, chlorophylls, and other components absorb light at different wavelengths, the spectrum data from EVOO samples are frequently complicated, making it difficult to identify and measure individual pigments.

Deconvolution models have become a potent tool for resolving overlapping spectral features in response to this difficulty. By dissecting the combined absorbance signal into its component parts, or deconvolution, precise pigment measurement is made possible. This method is especially helpful in the case of EVOO, as the spectra of carotenoids and chlorophylls frequently overlap, making direct measurement challenging. More accurate concentration estimations can be obtained by extracting the individual absorbance contributions of each color from the UV-Vis spectra using a deconvolution model [6].

Spectroscopy is among the scientific disciplines where ML has transformed data processing in recent years [7], [8]. Large and complicated datasets like spectroscopic data are a good fit for ML techniques, especially supervised learning models. A ML model can be trained with existing absorbance spectra and pigment concentrations to predict pigment concentrations from new spectral data. This method has the ability to analyze EVOO samples quickly and automatically, eliminating the requirement for human interpretation and improving pigment quantification accuracy. Moreover, by adding more training data, ML models can be enhanced over time and become more flexible to accommodate various EVOO samples and circumstances.

UV-Vis spectroscopy, deconvolution models, and ML work together to provide a potent, non-invasive way to examine the pigment content of EVOO. The deconvolution process will be optimized through the use of ML techniques, increasing the precision and resilience of the pigment concentration forecasts. In addition to offering estimations of pigment concentration, this integrated technique has the potential to enable real-time in-field analysis. The capacity to quickly evaluate oil quality through pigment analysis becomes more crucial as the market for premium EVOO grows. This research attempts to develop a dependable and effective method for pigment quantification in EVOO by utilizing ML and sophisticated spectrum analysis techniques, improving quality control and authenticity verification.

II. Literature Review

The field of olive oil fine assessment has seen a giant integration of advanced analytical techniques and ML strategies, which collectively push the boundaries of what may be achieved in terms of accuracy, performance, and practicality.

Venturini *et al.* [9] conducted an extensive study on EVOO oxidation under prolonged storage conditions, using UV absorption and total fluorescence spectroscopy to gather large datasets. They applied ML algorithms, including AdaBoost, Random Forest (RF), Logistic Regression, and Naïve Bayes, achieving over 90% classification accuracy in assessing oil quality based on fluorescence intensities at excitation wavelengths of 300 nm and 480 nm. However, they noted limitations in dataset representativeness, calling for broader sample diversity across different EVOO types and conditions. Future directions include developing portable, field-ready fluorescence-based devices for practical use.

Sanaeifar *et al.* [10] investigated ML applications in assessing Virgin Olive Oil (VOO) quality indices, focusing on pigment concentrations such as chlorophyll and carotenoids. Using a combination of dielectric spectroscopy and computer vision to capture color features in various color spaces, they tested algorithms like Artificial Neural Networks (ANN), Support Vector Machines (SVM), Bayesian networks, and multiple linear regression for quality prediction and classification. The Bayesian network achieved perfect accuracy, though challenges included extensive data preprocessing and potential model overfitting in complex setups. Future work suggests using larger, more diverse datasets and exploring deep learning models to improve robustness in pigment concentration predictions.

Venturini *et al.* [11] developed an affordable fluorescence sensor combined with various ML algorithms to assess EVOO quality. Using a dataset of fluorescence spectra from 27 samples categorized as EVOO, VOO, or lampante olive oil, they applied ANN, SVM, and RF models, with ANN and RF achieving 100% classification accuracy. This demonstrated ML's ability to streamline data analysis by reducing preprocessing and manual feature extraction. However, the study was limited by a narrow dataset and few quality categories. The authors recommend future work to expand sample variety and employ deep learning to analyze pigment concentrations with greater detail, highlighting the potential of fluorescence spectroscopy and ML in food quality management.

Borello *et al.* [12] introduced an alternative method: the usage of near-UV visible spectroscopy to quantify pigment concentrations in EVOO, inclusive of β-CAR, LUT, chlorophyll a (Chl-a), chlorophyll b (Chl-b), and Pheo-a. Their spectral deconvolution technique facilitated fast analysis, with splendid efficiency compared to traditional chromatography. regardless of its advantages, limitations were identified, including demanding situations in replicating the close-to-UV-vis spectra of clean EVOOs due to minor carotenoid interference. The researchers recommended enhancing their method with the aid of incorporating ML and deep mastering algorithms, which can refine spectral evaluation and improve pigment quantification accuracy.

Some other comparative study by Borello and Domenici [13] evaluated two close-to-UV-Vis spectroscopic methods for determining pigment degrees in EVOO. They contrasted the conventional absorbance-primarily based method with a mathematical deconvolution method, finding that the latter supplied more specific and dependable consequences, addressing shortcomings like underestimation located in older strategies. Have a look at the proposal that ML and deep-gaining knowledge may be integrated to similarly beautify analytical precision, especially via accounting for minor pigments and adapting the analysis for fresher oil samples.

Lazzerini and Domenici's [14] work analyzed the pigment concentrations in Tuscan EVOOs over special harvest years. With the aid of applying a novel mathematical evaluation of absorption spectra, they quantified four primary pigments,

noting widespread variation in pigment stages relying on climatic situations and harvest-specific elements. Their findings were reinforced with the aid of Principal Component Analysis (PCA), which distinguished between harvest years primarily based on pigment profiles. They advised that ML integration should facilitate extra robust spectral fact evaluation, helping cope with barriers inclusive of the overlook of sweet sixteen pigments.

Violino *et al.* [15] explored the geographical category of EVOO using an open-source VIS-NIR spectrophotometer mixed with artificial intelligence (AI). Analyzing ninety-two samples from Italy and different nations, they employed a synthetic neural community that categorized oils based totally on 288 spectral transmittance values with a ninety-four.6% accuracy price. In spite of this, challenges blanketed the small pattern size, impacting the model's reliability. hints for future paintings protected the use of large datasets and exploring extra spectral features, highlighting the capability of ML for greater nuanced pigment awareness evaluation.

In their study, Venturini *et al.* [16] revisited their technique of using a fluorescence sensor for first-class evaluation, this time specializing in an extra-widespread dataset of 540 spectra throughout 27 samples. Again, ANN and RF fashions stood out with 100% class accuracy. However, the look at mentioned that a broader illustration of oil kinds and similarly validated the usage of large datasets were wanted. The incorporation of deep getting to know ought to enhance those fashions, mainly for complex pigment attention analyses in various situations, demonstrating the convergence of ML and fluorescence spectroscopy as treasured for actual-international programs within the meals industry.

Violino *et al.* [17] also evaluated optoelectronic methods for sorting olives, which at once impacts EVOO best. Using an RGB optical sorting system and photograph evaluation, they performed 87% type accuracy for inexperienced olives, but confronted challenges with black olives (63.7% accuracy), largely because of visible imperfections like bruises. The authors proposed including spectral evaluation, which includes NIR sensors, and using ML and deep mastering to enhance detection precision and better examine pigment concentrations, advancing automated high-quality evaluation.

Moyano, Heredia, and Meléndez-Martínez [18] provided an extensive evaluation of olive oil pigments, emphasizing chlorophylls and carotenoids and their position in determining oil excellent and fitness blessings. They highlighted traditional analytical techniques, like high-performance liquid chromatography (HPLC) and spectrophotometry, at the same time as noting the restrictions of those strategies, including time-eating processes and subjective color checks. They proposed the use of ML algorithms to create extra-dependable pigment attention models, improving the evaluation technique's speed and objectivity and aligning with customer interest in nutritional transparency. Gyftokostas *et al.* [19] explored ML-type Greek EVOOs based totally on their starting place using spectroscopic strategies like laser-precipitated breakdown spectroscopy and absorption spectroscopy. The gradient-boosting set of rules accomplished awesome accuracy ranges (ninety-six% education, ninety-three. 8% validation). Barriers mentioned protected the need for advanced function selection and ability model enhancement through combining various information resources. The authors encouraged incorporating more sophisticated ML and deep studying techniques for more strong classification, reinforcing the intersection of AI with exceptional and authentic research. Jurinovich and Domenici [20] evolved a consumer-pleasant digital device referred to as EVOODec for analyzing UV-Vis spectra of EVOOs, specializing in pigment quantification. Their results, aimed toward academic use, showed fine student results and reinforced the tool's accessibility for non-experts. They highlighted the ability of further integrating ML to enhance analysis accuracy and cited that combining various spectral facts ought to enhance future fashions, advancing exceptional manipulation and academic methodologies. Lobo-Prieto *et al.* [21] used fluorescence spectroscopy paired with parallel thing analysis (PARAFAC) to look at VOO's pigment concentration modifications over garage. They correlated fluorescence information with HPLC measurements, indicating robust potential for ML programs to evaluate pigment concentrations in saved oil. They advocated developing ML fashions that integrate fluorescence records with chemical and sensory facts for a complete predictive approach, advancing industry requirements for freshness and satisfactory monitoring.

Arrizabalaga-Larra aga *et al.* [22] carried out extremely-HPLC and high-resolution mass spectrometry to evaluate Spanish EVOO pigments. They utilized multivariate data like PCA and partial least squares discriminant evaluation for local categories, looking at awesome pigment profiles encouraged by environmental elements. While powerful, their examine did not combine ML, suggesting destiny studies may want to follow AI to investigate complicated pigment facts more deeply, reaping rewards for authenticity efforts. Lazzerini, Cifelli, and Domenici [23] authored a chapter on the importance of pigment concentrations for EVOO exceptionality and authenticity. They discussed chromatographic and spectroscopic methods but talked about their drawbacks, along with hard work-in-depth pattern training. The authors counseled that ML ought to streamline pigment analysis, providing real-time class based totally on full-size spectral datasets, and improving industry practices. Fathy *et al.* [24] investigated the usage of bodily characteristics like coloration, viscosity, and refractive index for assessing EVOO nice through photo analysis and chemometric strategies. With the aid of PCA and Orthogonal Partial Least Squares - Discriminant Analysis (OPLS-DA), they differentiated oils from diverse origins, achieving high type accuracy. The look at referred to environmental influences on pigment awareness and recommended that destiny ML integrations should enhance predictive models, refining quality manipulation further.

Ultimately, Gucciardi *et al.* [25] combined optical fluorescence sensors with ANNs to assess EVOO first-rate. They examined numerous neural community architectures, and locating a Convolutional Neural Network (CNN) finished an 82% classification charge. challenges protected pattern size and variability in chemical residences. Future work cautioned dataset enlargement and deeper ML feature exploration, pushing the capacity of AI to decorate pigment attention evaluation

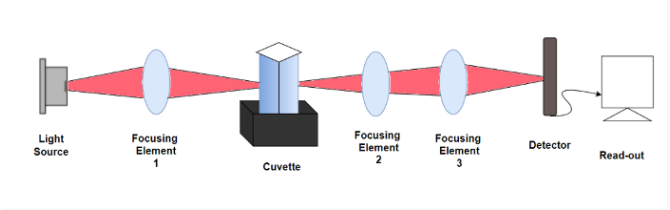

Fig. 1: Schematic diagram of the portable UV-Vis spectroscopic setup for EVOO analysis: (a) Broad-spectrum halogen light source (380-720 nm), (b) Plano-convex focusing lens 1, (c) Plano-concave diffusing lens, (d) Plano-convex focusing lens 2, (e) Temperature-controlled sample chamber with 1 cm quartz cuvette, (f) CMOS detector array, (g) Raspberry Pi 4B controller, and (h) 3D-printed housing with integrated cooling. The optical path is optimized for maximum sample interaction while minimizing stray light interference.

and fine differentiation in olive oil. In precis, leveraging gadgets, gaining knowledge of, and advanced spectroscopic strategies extensively enriches pigment concentration analysis in EVOO, providing a sturdy framework for extra-green, scalable, and specific best evaluation. These methodologies no longer only help conventional analytical techniques but also open new avenues for innovation in meals technological know-how and industry practices.

III. Materials and Methods

A. UV-Vis Spectroscopy Hardware

The standard UV-Vis spectroscopy setup was used in the earlier methods [6] to determine pigment concentrations in EVOO by measuring light absorbance in the 380–720 nm region. The absorbance peaks of carotenoids and chlorophylls, which add to the color, flavor, and nutritional content of EVOO, are captured by this carefully chosen wavelength range. Spectrophotometers that are sold commercially are frequently big, expensive, and trained staff intensive. The portable UV-Vis spectroscopic apparatus is intended to be flexible instrument for quality control and analysis in a range of contexts due to its small size and field-compatible design. While a portable UV-Vis spectrometer offers significant utility and convenience for field-based spectroscopic analysis, it can be relatively expensive, which may limit its accessibility for some users. These constraints are addressed by the creation of a portable apparatus, which makes it possible to conduct accurate on-site EVOO analysis. Decisions on the nutritional and commercial worth of the oil can be informed by real-time data gathering on pigment concentrations, which makes this device particularly useful for quality control and research. The setup consists of several key components arranged to ensure accurate light measurement. Light from a source that spans the necessary wavelength range is used to start the process. Three focusing elements are included in the optical path that this light travels through: one plano-concave lens (Focusing Element 2) and two plano-convex lenses (Focusing Elements 1 and 3). The light is focused and directed toward the sample holder and detector by the plano-convex lenses. By slightly diffusing the light, the plano-concave lens in the center (focusing element 2) contributes to the uniform dispersion of light. By reducing stray light and guaranteeing a well-focused light path, this optical configuration increases measurement accuracy. The EVOO sample-containing cuvette is positioned in the focused light's path. Depending on their concentration, the pigments in EVOO absorb particular light wavelengths, lowering the intensity of light that is transmitted. The arrangement optimizes light-sample interaction by placing the cuvette at the center of the light path. By using a typical path length of 1 cm, Beer's Law can be applied for further study. The light travels through the sample and then reaches a detector, which logs the intensity drop brought on by the pigments' absorption. Because of its sensitivity across the UV-Vis spectrum, the detector can identify even minute variations in absorbance, which are correlated with trace pigment concentrations. Each sample's absorbance spectrum is produced using this data. The Raspberry Pi Model 4b microcomputer is in charge of data collecting and analysis. Because the complete system is contained in a specially designed 3D-printed container, stability is guaranteed, outside light interference is reduced, and portability is improved. The device is also inexpensive and adaptable due to its 3D-printed framework, which makes it ideal for field use. To ascertain unknown pigment amounts, the software employs a linear regression to a calibration curve based on established standards after processing absorbance values in real time.

B. Spectral Data Collection, Preprocessing, and Feature Extraction

For this study, we analysed five distinct oil samples to evaluate the robustness of our method across various oil types: Standard EVOO, Fresh EVOO, Maize seed oil, Monocultivar Frantoio EVOO, and Rapeseed oil. These samples were chosen to represent a range of oil compositions, from high-quality EVOOs to other vegetable oils, allowing us to test the versatility of our analytical approach [2], [13]. We employed UV-Vis spectroscopy to collect absorbance data for each oil sample [12]. The spectral acquisition process followed a standardized protocol to ensure consistency and reliability of the data. We focused on the wavelength range of 390-720 nm, which encompasses the visible spectrum and near-UV region. This range is particularly relevant for capturing the absorbance patterns of key pigments in olive oil, including chlorophylls and carotenoids [18].

To optimize our spectral data for ML analysis, we implemented a comprehensive preprocessing and feature extraction pipeline. This process, detailed in Algorithm 1, consists of five main stages designed to enhance data quality, consistency, and informativeness across all samples.

This initial stage ensures consistency across all samples by standardizing column names, converting wavelength values to a numeric format, and removing any rows with missing or corrupted data. We also implement outlier detection and removal to enhance data quality. This step is crucial for maintaining data integrity throughout the analysis process. We focus on the spectral region between $\lambda_{min} = 390$ nm and

Algorithm 1 Spectral Data Preprocessing and Feature Extraction

Require:
$\mathcal{D}_{raw}$: Raw spectral data
ε_{ref}: Reference pigment extinction coefficients
λ_{min}, λ_{max}: Minimum and maximum wavelengths
Ensure:
$\mathcal{D}_{opt}$: Optimized dataset for machine learning analysis
procedure SPECTRALPREPROCESSING ($\mathcal{D}_{raw}$, ε_{ref}, λ_{min}, λ_{max})
$\mathcal{D}_{clean} \leftarrow$ CLEANANDSTANDARDIZE ($\mathcal{D}_{raw}$) ▷ Remove outliers and standardize format
$\mathcal{D}_{filtered} \leftarrow$ FILTERWAVELENGTHRANGE ($\mathcal{D}_{clean}$, λ_{min}, λ_{max}) ▷ Select relevant spectral range
$\mathcal{D}_{corrected} \leftarrow$ BASELINECORRECTION ($\mathcal{D}_{filtered}$) ▷ Apply baseline correction
$\varepsilon_{norm} \leftarrow$ NORMALIZEEXTINCTIONCOEFFICIENTS (ε_{ref}) ▷ Normalize reference coefficients
$\mathcal{D}_{opt} \leftarrow$ CONSTRUCTFEATUREVECTOR ($\mathcal{D}_{corrected}$, ε_{norm}) ▷ Extract features
return $\mathcal{D}_{opt}$

$\lambda_{max} = 720$ nm. This range encompasses the visible spectrum and near-UV region, which is particularly informative for analyzing chlorophylls and carotenoids in olive oil. By filtering the data to this specific range, we reduce noise and focus on the most relevant spectral information.

To minimize the impact of background noise and improve the signal-to-noise ratio, we applied a baseline correction by subtracting the minimum absorbance value from each spectrum. This step allows for more accurate comparisons between samples by eliminating systematic offsets in the spectral data [20]. We utilize a reference dataset (ε_{ref}) containing the extinction coefficients of eight key pigments commonly found in olive oil: Chl-a and Chl-b, Pheo-a and Pheo-b, β-CAR, LUT, NEX, and an unspecified triene [3], [22]. Our normalization process ensures non-negative coefficients, scales each pigment's extinction coefficient relative to its maximum value, and creates a consistent scale across different pigments [23]. This normalization is crucial for maintaining the relative importance of each pigment in the subsequent analysis.

The final stage combines the processed spectral data ($\mathcal{D}_{corrected}$) with the normalized extinction coefficients (ε_{norm}) to create a comprehensive input dataset for our ML model. This approach encapsulates both the experimental absorbance data and the reference pigment information, providing a rich feature set for analysis. The resulting optimized dataset ($\mathcal{D}_{opt}$) serves as input for our ML model, encapsulating the essential spectral and pigment information in a format conducive to advanced analysis.

C. Traditional Deconvolution Method

As a baseline for comparison, we implemented the traditional deconvolution approach described by Domenici *et al.* [12]. This method involves analysing the entire UV-Vis absorption spectrum to extract pigment concentrations through matrix operations and eigenvector calculations. Algorithm 2 presents the key steps of this process.

Algorithm 2 Traditional Deconvolution Method

Compute overlap matrix of reference spectra
Diagonalize overlap matrix
Compute eigenvectors for new base
Calculate Spectral Variance (SV) coefficients
Compute pigment concentrations
Reconstruct spectrum and calculate residuals

The method begins with the input of the experimental EVOO spectrum and reference pigment spectra. It then computes the overlap matrix S of reference spectra, diagonalizes it to obtain eigenvalues and eigenvectors, and calculates new basis eigenvectors. This is followed by the computation of SV coefficients and pigment concentrations. Finally, the algorithm reconstructs the calculated spectrum and determines residuals. This approach allows for the simultaneous quantification of multiple pigments by leveraging the entire spectral information. While it has shown good accuracy in previous studies [12], it can be computationally intensive and may face challenges with highly complex or noisy spectra.

D. Regularized Adaptive Deconvolution (RAD) Model

Building upon the traditional deconvolution approach, we developed a ML-based RAD model to enhance the accuracy and efficiency of pigment concentration estimation in olive oil samples.

1) Model Architecture: The RAD Model is implemented as a neural network designed to learn pigment concentrations directly from spectral data. The core of the model is a learnable parameter vector representing the concentrations of different pigments in the oil sample. The model architecture can be described as follows:

$$c = \text{ReLU}(w) \tag{1}$$

where w is the learnable parameter vector and ReLU (Rectified Linear Unit) is an activation function that ensures non-negative concentration values, which is physically meaningful in the context of pigment concentrations [26]. The predicted absorbance spectrum is then computed as:

$$A_{calc} = (b \cdot c^T \varepsilon) \tag{2}$$

where b is the optical path length, c is the vector of learned concentrations, and ε is the matrix of normalized extinction coefficients for the pigments under consideration.

2) Loss Function and Optimization: The model is trained to minimize the Mean Squared Error (MSE) between the calculated absorbance spectrum and the experimental spectrum:

$$L_{MSE} = \frac{1}{n} \sum_{i=1}^{n} (A_{exp,i} - A_{calc,i})^2 \tag{3}$$

where n is the number of wavelengths in the spectrum, $A_{exp,i}$ is the experimental absorbance at wavelength i, and

Algorithm 3 Training Procedure for RAD Model

Initialize model parameters randomly using seed
Initialize ADAM optimizer and `REDUCELRONPLATEAU` scheduler
best_loss $\leftarrow \infty$
no_improve_count $\leftarrow 0$
for epoch = 1 to num_epochs **do**
  $A_{calc} \leftarrow MODEL(\varepsilon)$
  $mse\_loss \leftarrow MSE(A_{calc}, A_{exp})$
  $l2_{loss} \leftarrow \lambda \cdot l2_{loss}$
  $loss \leftarrow mse\_loss + l2_{loss}$
  Compute gradients of loss
  Apply gradient clipping
  Update model parameters using ADAM optimizer
  Update learning rate using scheduler
  if $loss < best\_loss$ **then**
    $best\_loss \leftarrow loss$
    $no\_improve\_count \leftarrow 0$
  else
    $no\_improve\_count \leftarrow no\_improve\_count + 1$
  end if
  if $no\_improve\_count \geq patience$ **then**
    break
  end if
end for
return trained model

$A_{calc,i}$ is the calculated absorbance at the same wavelength. To prevent overfitting and encourage more stable solutions, we incorporate L2 regularization into the loss function [28]. This addition helps to constrain the model parameters, leading to better generalization, especially when dealing with complex or noisy spectra. The modified loss function is:

$$L = L_{MSE} + \lambda \|w\|_2^2 \tag{4}$$

where λ is the regularization parameter, and $\|w\|_2^2$ is the L2 norm of the model parameters.

For optimization, we employ the ADAM (Adaptive Moment Estimation) algorithm [27], which adapts the learning rate for each parameter and incorporates momentum to help overcome local minima. Additionally, we implement the `REDUCELRONPLATEAU` scheduler, which dynamically adjusts the learning rate during training based on the model's performance [29]. This technique allows for more efficient optimization, particularly in the later stages of training when fine-tuning is crucial. These enhancements address key challenges in spectral analysis, such as the sensitivity to noise and the potential for overfitting, which are common issues in traditional deconvolution methods [30].

E. Training Procedure and Evaluation

1) Training Algorithms: The RAD Model is initialized with random parameters using a fixed seed for reproducibility. It incorporates L2 regularization into the loss function, employs gradient clipping to prevent extreme parameter updates, and utilizes the ReduceLROnPlateau scheduler for adaptive learning rate adjustment. The model also implements an early stopping mechanism to prevent overfitting and unnecessary computation [31].

2) Evaluation Methodology: The evaluation of both the traditional and RAD models focuses on three key aspects:

1) Coefficient of determination (R^2) between experimental and calculated spectra
2) Visual comparison of spectral reconstructions
3) Estimated pigment concentrations

The R^2 value quantifies the goodness of fit, providing a numerical measure of how well the models capture the variance in the experimental data. Visual comparisons allow for a qualitative assessment of the models' ability to reproduce key spectral features, such as absorption peaks and band shapes. Finally, the estimated pigment concentrations are compared across models and with literature values for typical EVOO compositions [3], [14].

This comprehensive evaluation approach was applied to five distinct oil samples: standard EVOO, fresh EVOO, maize seed oil, monocultivar Frantoio EVOO, and rapeseed oil. This diverse set of samples enabled a thorough assessment of the models' performance across various oil compositions and pigment profiles, providing insights into their potential for rapid, non-destructive pigment analysis in the food industry [2], [13], [15], [24].

F. Interpretability Techniques

To validate our results and gain insights into underlying physical and chemical processes, we implemented several advanced interpretability techniques for the RAD model. These techniques not only help validate our model's predictions against known properties of olive oil pigments but also offer new insights into the complex relationships between pigment concentrations and absorption spectra in various types of oils [34].

One of the primary methods we employed is Integrated Gradients [35]. This technique attributes the prediction of a deep network to its input features, providing a measure of feature importance. In our context, it shows the significance of each wavelength for different pigments in the UV-Vis spectrum. The Integrated Gradients for an input x and baseline x^0 is defined as:

$$IG_i(x) = (x_i - x_i') \cdot \int_{\alpha=0}^{1} \frac{\partial F(x' + \alpha(x - x'))}{\partial x_i} \, d\alpha \tag{5}$$

where F is the model's output. This method allows us to understand which spectral regions are most influential in determining the concentration of specific pigments.

We also utilized Saliency Maps [36], which reveal the model's sensitivity to each pigment across different wavelengths. The saliency S_{ij} for input feature x_{ij} is computed as:

$$S_{ij} = \left| \frac{\partial y}{\partial x_{ij}} \right| \tag{6}$$

Algorithm 4 Model Interpretation

Require: Trained model M, input data X, experimental absorbance A_{exp}, wavelengths W
Ensure: Visualizations of model interpretability
1: $IG \leftarrow$ COMPUTEINTEGRATEDGRADIENTS (M, X)
2: $S \leftarrow$ COMPUTESALIENCYMAP (M, X)
3: $A_{calc} \leftarrow$ M (X)
4: PLOTABSORBANCESPECTRA(A_{exp}, A_{calc}, W)
5: PLOTINTEGRATEDGRADIENTSHEATMAP (IG, W)
6: PLOTSALIENCYMAP (S, W)

where y is the model output. This technique helps identify which pigments most strongly influence predictions at various points in the spectrum.

This algorithm is applied to the RAD Model. Our implementation leverages the Captum library [37], which provides state-of-the-art tools for model interpretability in PyTorch. The use of this library ensures that our interpretability methods are efficiently implemented and consistent with current best practices in the field.

The integration of these interpretability techniques enhances the transparency and reliability of our ML-based method for pigment concentration prediction in EVOO using UV-Vis spectroscopy. By providing a detailed view of how our models arrive at their predictions, we not only validate our approach but also contribute to a deeper understanding of the spectral characteristics of different pigments in olive oil and other vegetable oils. This comprehensive interpretability framework allows for a more nuanced analysis of pigment concentrations, potentially leading to improved quality control processes in the olive oil industry and more accurate authentication methods. Furthermore, the insights gained from these techniques may inform future research directions in spectroscopic analysis of complex organic mixtures, extending beyond olive oil to other areas of food science and analytical chemistry.

IV. Results and Discussion

Two methods were used in our study to analyse the pigment concentrations in different oil samples, a traditional deconvolution model [12] and a ML-based RAD Model. Standard EVOO, fresh EVOO, maize seed oil, monocultivar frantoio EVOO, and rapeseed oil were the five oil samples to which we applied these techniques. Estimates of pigment concentration and spectral reconstruction performance were the two primary areas of analysis.

A. Spectral Reconstruction Performance

1) Comparison of R² values: Both models demonstrated excellent spectral reconstruction capabilities across all samples, as evidenced by the high coefficient of determination (R^2) values presented in Table I.

The consistently high R^2 values (>0.99) for both models indicate that they explain over 99% of the variance in the experimental data for all samples. This level of accuracy aligns with or exceeds that reported in previous studies using spectroscopic methods for olive oil analysis [15], [24]. Notably,

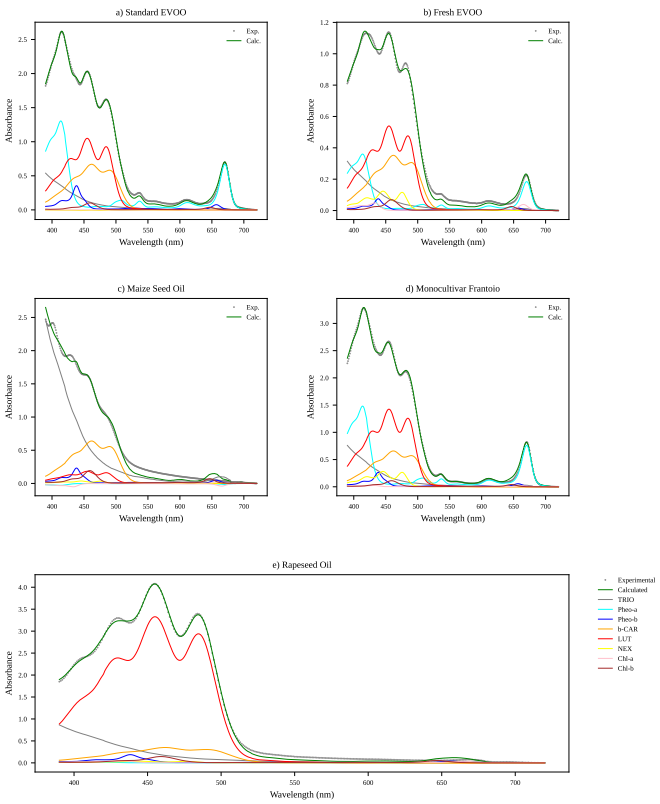

Fig. 2: Spectral reconstruction and individual pigment contributions using traditional deconvolution analysis of UV-Vis spectra for: (a) Standard EVOO, (b) Fresh EVOO, (c) Maize Seed Oil, (d) Monocultivar Frantoio EVOO, and (e) Rapeseed Oil. Dotted points represent experimental data, solid lines show calculated total spectrum and individual pigment contributions.

TABLE I: R^2 Values for Spectral Reconstruction

Sample	Traditional Model	RAD Model
Standard EVOO	0.998909	0.998976
Fresh EVOO	0.995542	0.997664
Monocultivar Frantoio	0.992892	0.992894
Maize Seed Oil	0.999351	0.999351
Rapeseed Oil	0.996130	0.998951

the RAD model showed slight improvements in R^2 values for most samples, with the most significant enhancement observed for Rapeseed Oil (from 0.996130 to 0.998951).

2) Visual comparison of reconstructed spectra: The spectral reconstructions from both models demonstrate excellent agreement with experimental data, though with distinct characteristics. Figure 2 shows the traditional deconvolution results following Borello et al.'s approach [12], highlighting individual pigment contributions through colored spectral components. For Standard EVOO (Figure 2(a)), distinct peaks are observed at 400-500 nm (carotenoids) and 670 nm (chlorophylls), aligning with the characteristic absorption patterns reported by Moyano et al. [18]. Fresh EVOO (Figure 2(b)) shows lower overall absorbance but maintains similar spectral features, consistent with pigment evolution patterns observed by Borello and Domenici [13].

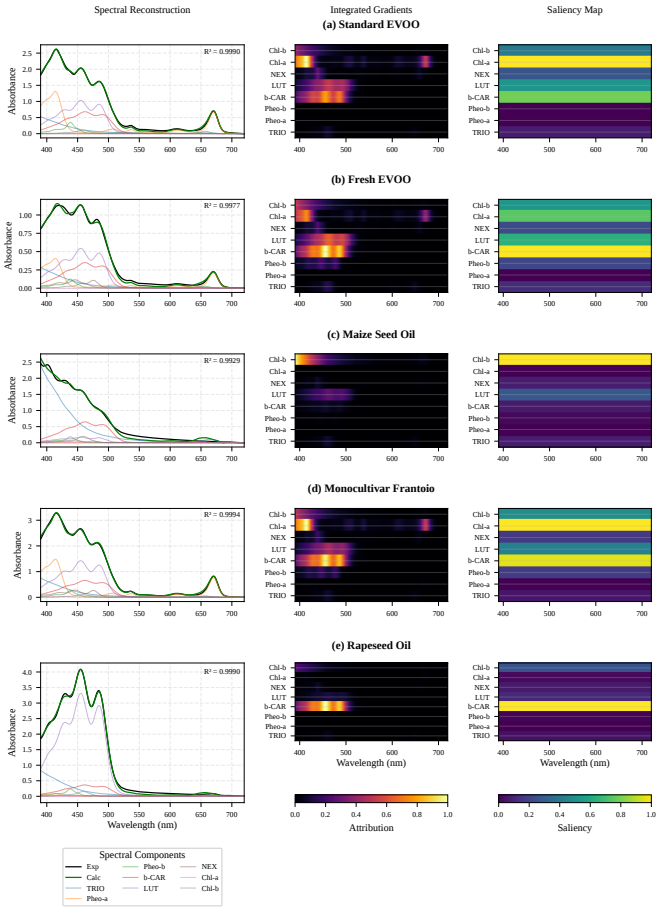

Fig. 3: Comparative analysis using the RAD model showing (left) Spectral Reconstruction with experimental data and calculated fits, (middle) Integrated Gradients heatmaps indicating wavelength-specific pigment contributions, and (right) Saliency Maps demonstrating model sensitivity patterns for: (a) Standard EVOO, (b) Fresh EVOO, (c) Maize Seed Oil, (d) Monocultivar Frantoio EVOO, and (e) Rapeseed Oil.

Figure 3's left column presents the RAD model's reconstructions, displaying comparable accuracy with enhanced resolution of subtle spectral features, particularly in regions where traditional methods face challenges [12]. The model excels in capturing complex overlapping regions in Standard EVOO (Figure 3(a)) and Fresh EVOO (Figure 3(b)), demonstrating improvements over traditional spectroscopic techniques [2]. Notable advancements are observed in the Rapeseed Oil analysis (Figure 3(e)), where the RAD model better resolves the intricate spectral features between 450-500 nm, addressing limitations previously identified in conventional approaches [14]. Both models achieve excellent fits across all samples, though the RAD model demonstrates superior handling of spectral overlap and baseline stability, consistent with recent improvements in spectroscopic analysis methods [15], [24].

B. Pigment Concentration Estimates

Table II presents a comprehensive comparison of pigment concentration estimates (in mg/kg) obtained from both the traditional deconvolution model and the RAD model across five diverse oil samples.

The results reveal intriguing patterns and differences between the two models. In Standard EVOO, both models identified Pheo-a as the dominant pigment, with the RAD model generally estimating slightly higher concentrations for most pigments. Fresh EVOO analysis showed notable differences in carotenoid profiles between the models, with the RAD model suggesting higher LUT concentrations. Interestingly, both models indicated the absence of Chl-a in fresh EVOO, which aligns with expected degradation patterns in olive oil [2]. The analysis of Maize Seed Oil demonstrated strong agreement between the models, with β-CAR emerging as the dominant pigment. Monocultivar Frantoio EVOO exhibited excellent consistency between the two models, showcasing only minor variations across all pigments. However, the most significant disparities were observed in Rapeseed Oil, where the RAD model proposed markedly different concentrations for several pigments, particularly higher LUT and lower β-CAR and NEX compared to the traditional model.

A critical observation is the occurrence of negative concentration values in the traditional model's estimates, particularly for pigments like NEX in Standard EVOO (-0.052 mg/kg) and Chlorophyll a (Chl-a) in Maize Seed Oil (-0.438 mg/kg). These negative values are physically impossible and represent a limitation of the traditional deconvolution approach. In contrast, the RAD model consistently produced non-negative concentration estimates across all samples, demonstrating its ability to enforce realistic constraints on the predicted values. This improvement is attributed to the use of the ReLU activation function in the RAD model, which ensures non-negative outputs [26]. The RAD model's realistic concentration estimates, especially in complex samples like Rapeseed Oil, suggest its enhanced capability to differentiate between closely related pigments and handle complex spectral interactions. These results align with previous studies on pigment compositions in various oil types [3], [14], [22] while highlighting the potential improvements offered by ML-enhanced approaches in spectral analysis and pigment quantification.

C. Model Interpretation Results

The RAD model's interpretability analysis through Integrated Gradients and Saliency Maps reveals comprehensive insights into pigment-wavelength relationships across different oil types. The Integrated Gradients analysis (Figure 3, middle column) demonstrates distinct wavelength-specific patterns that validate our model's accuracy in pigment identification. For Standard EVOO (Figure 3(a)), strong attributions are observed in the 400-500 nm range for carotenoids and at 670 nm for chlorophyll-related pigments, aligning with established spectral characteristics [18]. This pattern is particularly pronounced in Monocultivar Frantoio (Figure 3(d)), where the model effectively captures the complex interplay between different pigment classes.

The Fresh EVOO analysis (Figure 3(b)) reveals distinct attribution patterns in the carotenoid region, consistent with degradation patterns documented by Borello et al. [2]. This

TABLE II: Pigment Concentration Estimates (mg/kg) for Different Oil Samples Using Traditional and RAD Models

Pigments	Standard EVOO		Fresh EVOO		Monocultivar EVOO		Maize Seed Oil		Rapeseed Oil	
	Trad.	RAD	Trad.	RAD	Trad.	RAD	Trad.	RAD	Trad.	RAD
Pheo-a	10.755	10.906	2.969	3.375	12.212	12.376	-0.239	0.000	0.230	0.665
Pheo-b	1.935	1.936	0.408	0.697	1.438	1.465	1.264	1.018	1.019	1.316
β-CAR	2.983	3.070	1.569	1.576	2.933	2.970	2.850	2.920	1.561	1.653
LUT	4.953	4.922	2.545	2.594	6.723	6.793	0.865	0.842	15.701	15.793
NEX	-0.052	0.000	0.647	0.610	1.478	1.504	0.194	0.297	0.193	0.165
Chl-a	-0.022	0.015	0.422	0.000	0.216	0.214	-0.438	0.000	0.384	0.000
Chl-b	0.869	0.905	0.586	0.615	0.944	0.952	1.641	1.683	1.220	1.310
Total	21.421	21.754	9.146	9.467	25.944	26.273	6.136	6.761	33.273	20.902

observation is further supported by the pigment concentration estimates in Table II, where the RAD model shows improved accuracy in quantifying subtle changes in carotenoid profiles, particularly for LUT (2.594 mg/kg) compared to the traditional model (2.545 mg/kg).

The Saliency Maps (Figure 3, right column) provide additional validation of our model's capabilities. For EVOO samples, heightened sensitivity to chlorophyll-related pigments (Chl-a, Chl-b) in the 650-700 nm range aligns with findings from Lazzerini and Domenici [14]. The model's ability to differentiate between closely related pigments is evidenced by the distinct sensitivity patterns for β-CAR and LUT in the 400-500 nm region, a capability previously limited in traditional approaches [12].

A significant advancement is demonstrated in the analysis of non-EVOO samples. Maize Seed Oil (Figure 3(c)) shows distinctive patterns focused primarily in the carotenoid region, while Rapeseed Oil (Figure 3(e)) exhibits unique sensitivity distributions for LUT. These results align with compositional analyses reported by Borello and Domenici [13] and are supported by our concentration estimates showing physically realistic, non-negative values across all pigments, addressing a key limitation of traditional methods.

The RAD model's superior performance is particularly evident in challenging cases. For instance, in Rapeseed Oil analysis, where traditional methods struggled with negative concentration values, our model maintains physically meaningful estimates while achieving higher R^2 values (0.998951 versus 0.996130). This improvement is attributed to the model's novel architecture incorporating ReLU activation [26] and L2 regularization, enabling more robust handling of complex spectral interactions [34].

These results, supported by both interpretability techniques and quantitative measurements, demonstrate the RAD model's advancement over traditional methods. The model not only provides more accurate pigment quantification but also offers deeper insights into pigment-specific spectral contributions, establishing a new benchmark for spectroscopic analysis in oil authentication and quality control [19], [25].

V. Conclusion

This study demonstrates the significant advancement in spectroscopic analysis through our new ML based RAD model, representing a key evolution in ML applications for olive oil authentication and quality control. Our comparative analysis with traditional deconvolution methods revealed the RAD model's superior capabilities across diverse oil samples, consistently achieving high accuracy in spectral reconstruction (R^2 ¿ 0.99) while addressing fundamental limitations of conventional approaches. The model's integration of ReLU activation functions and L2 regularization proved particularly effective in eliminating physically impossible negative concentration estimates, a persistent challenge in traditional methods [12], [13]. This was notably demonstrated in complex samples like rapeseed oil, where the RAD model achieved superior accuracy (R^2 = 0.998951) compared to traditional approaches (R^2 = 0.996130). The model's ability to maintain physically meaningful concentration estimates while improving spectral reconstruction aligns with recent advancements in spectroscopic analysis [15], [24].

Our implementation of advanced interpretability techniques, including Integrated Gradients [35] and Saliency Maps [36], provides unprecedented insight into pigment-wavelength relationships. The visualization of these relationships validates established spectral characteristics [18] while offering new perspectives on pigment interactions, particularly in the carotenoid (400-500 nm) and chlorophyll (670 nm) regions. This enhanced interpretability framework addresses a critical gap in spectroscopic analysis methods [34], making the RAD model particularly valuable for real-world applications. The model's consistent performance across various oil types, from standard EVOO to complex mixtures like rapeseed oil, demonstrates its robust applicability in industrial settings. The combination of accurate quantification, enhanced interpretability, and reliable performance establishes a new benchmark for non-destructive analysis in food science [19], [25]. Looking ahead, this approach opens new avenues for rapid, accurate quality control in olive oil production and authentication, advancing the field's analytical capabilities beyond traditional spectroscopic methods. The RAD model's success in combining ML with spectroscopic analysis suggests promising applications beyond olive oil analysis, potentially extending to other areas of food science and analytical chemistry where complex spectral interactions require sophisticated interpretation [7], [8]. This work demonstrates how advanced ML techniques can enhance traditional analytical methods while maintaining interpretability and practical applicability, contributing to the broader evolution of food quality assessment techniques.

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