Artificial Intelligence in Analytical Spectroscopy, Part II: Examples in Spectroscopy

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In Part I (February 2023) of this two-part series on artificial intelligence (AI), and its subfield machine learning (ML), we presented the variety of chemometric algorithms used to compare AI, ML, and chemometrics. These algorithms included those used for classification, regression, clustering, ensemble learning, signal processing, and component analysis. Now, in Part II, we discuss the applications of AI to electronic and vibrational spectroscopy. We also touch on some applications of deep learning (DL), which is a subfield of machine learning where more complex artificial neural networks (ANNs) with more hidden layers are used. This column article includes a number of selected references that discuss the application of AI in analytical chemistry and in molecular spectroscopy. We give a few early and late examples of AI and ML as applied to different vibrational spectroscopy methods, such as Raman, infrared (FT-IR), near-infrared (NIR), and ultraviolet–visible (UV-vis) spectroscopic techniques. This article is intended only as a sampling of the numerous research manuscripts addressing this subject.

Since 2010, there has been a rapid growth in the application of

applications. AI, when properly applied and evaluated using domain knowledge, is a useful tool for routine processing of large quantities of data and for assisting humans in performing routine or repetitive tasks with high repeatability and accuracy. AI also has significant potential for automating well-understood complex tasks, and for advancing discovery of new molecules and materials by integrating and combining known physical science principles with new innovative concepts and approaches. We bring to the reader's attention that, strictly speaking, AI does not always indicate the use of neural networks. Neural networks are one of the many techniques used in AI, but they are not the only ones. AI encompasses a wide range of techniques and approaches, including rule-based systems, decision trees, genetic algorithms, and others.

General Trends for AI in Analytical Chemistry

AI use is increasing rapidly for analytical chemistry applications. Review articles are a useful starting place to explore this growing field. A tutorial review of AI applications in analytical chemistry was published in 2021 (1). This review discusses the application advances in computer processing power and algorithms of AI in chemistry for creating new compounds and novel approaches in organic synthesis, drug discovery, and design of materials. The authors report that the use of AI to support analytical purposes has been mostly limited to data analysis methods, such as image recognition, vibrational spectroscopy, and mass spectrometry. The review describes basic concepts related to implementing AI, and states that there are many new opportunities for allying AI technology to spectroscopy and separation science as well as sensor output and design.

Another valuable review paper describes the trends in AI and the relationship of machine learning to chemometrics (2). In fact, this paper refers to chemometrics as an AI-based method, along with machine learning and deep learning (DL, a subfield of machine learning [ML]). The paper proposes that AI methods lead to an improved understanding of data. The authors state that AI, when used to its full extent, allows improved insight into the various processes, interactions, and characteristics of sample analysis data. The review highlights that AI-based techniques have been applied to chemical data since the 1970s and many AI approaches were being used by 2020. The paper specifically describes inverse modeling, preprocessing methods, and data modeling techniques as applied to spectral and image analysis for several analytical techniques.

AI in Vibrational Spectroscopy

Vibrational spectroscopy techniques, such as Fourier transform infrared (FT-IR) and Raman spectroscopy, have been demonstrated to be highly successful analytical methods and

have proven to be low cost, require minimum sample preparation, be non-destructive, and yield highly valuable chemical information. There is a requirement for improvement and automation in data processing for classification and visualization of spectrochemical data measured from biological and medical samples. Multivariate classification is useful for assigning unknown samples to predefined groups and for information extraction from data. For this purpose, a tutorial article, representing the prerequisite algorithm requirements for machine learning approaches, has been published to demonstrate multivariate classification analysis using near-infrared (NIR), FT-IR, and Raman spectroscopy data (3). This paper highlights such steps as data preprocessing, data selection, feature extraction, classification, and model validation. These mathematical processes are essential for computation of practical spectrochemical classification models intended for analysis of biological samples.

A paper demonstrated that convolutional neural networks (CNNs), a basic AI and ML tool, can be used to effectively classify vibrational spectroscopy data as well as to identify important spectral regions (4). CNNs are capable of image classification, and can be used to learn or define various visual interpretations of spectroscopic data. CNNs are able to reduce the requirements for rigorous data preprocessing, and are able to identify the most important spectral regions for analyzing the desired spectral features of interest. Spectroscopic data is most often preprocessed as part of the chemometric modeling work. Such preprocessing steps include various types of baseline correction, scatter correction, noise reduction or removal, feature selection, derivative processing, and other steps, which are applied to the spectra prior to model building. As a standard practice, preprocessing has traditionally been considered essential for optimizing standard chemometric models. A simple CNN architecture, using a single convolutional layer (shallow CNN), has demonstrated improved performance as compared to standard classification algorithms such as partial least squares (PLS) regression. Classification accuracy for CNN vs. PLS was reported to be 86% vs 62%, respectively, for non-preprocessed test data, and 96% and 89%, respectively, for preprocessed data. The CNN algorithm was also able to identify important spectral regions, in order to assist in qualitative interpretation of classification results.

General Spectroscopic Applications of AI

Early work in implementing AI for spectroscopic applications described the identification of polyatomic molecules from their molecular spectra (5). This research concluded that AI systems provided one of the most promising potential developments for the future of analytical molecular spectroscopy, noting that AI systems presented a more dynamic analytical solution set. It was reported that AI systems are able to compare measured

spectra to computer-generated spectra, rather than just compare measured spectra to an archived spectral database. Such an AI approach offers more potential than manual methods to extract additional information from spectral analysis experiments.

In a series of papers, Luinge and colleagues have described the development of an AI expert system for spectral interpretation and for the elucidation of chemical structures from combined spectroscopic data (EXSPEC) (6–9). These papers describe the rationale and programming involved in creating such a system for interpretation of infrared, mass, and nuclear magnetic resonance (NMR) spectra for an earlier generation of computer systems.

In research to better connect Raman spectroscopy measurements of biomedical and clinical samples to medical diagnosis and decision-making, an AI system was designed as a way to understand the chemical pathways and the progression of disease (10). This approach has potential use for the future of personalized medicine. The initial stages of this AI system were designed to optimize spectral preprocessing in order to reduce noise, fluorescence and baseline effects, while employing the use of chemometrics. Specifically, this research analyzed breast cancer tissue samples using Raman spectroscopy combined with principal component (PCA) and linear discriminate analysis (LDA). For this work, tissue microarray (TMA) breast biopsies were classified into multiple groups, such as luminal A, luminal B, HER2, and triple negative subtypes. The classification accuracy results of applying the AI system to the Raman spectra, which contains chemical information on tissue lipid, collagen, and nucleic acid content, were 70%, 100%, 90%, and 96.7% for luminal A, luminal B, HER2, and triple negative subtypes, respectively. This result is quite encouraging for further disease tissue classification research.

Because vibrational spectroscopic techniques have shown significant progress in assessing biomedical samples, they are being further investigated using automated and AI data processing. When properly implemented, AI is capable of identifying and connecting meaningful chemical and diagnostic relationships for clinical samples measured using infrared or Raman spectroscopy. A special article assesses the current use of AI in biomedical vibrational spectroscopy applications (11).

AI in Raman Spectroscopy

ML, as a subfield of AI, is being used to extract, connect, and summarize information from large and complex analytical datasets for separation science, mass spectrometry, NMR, and atomic and molecular spectroscopy. The advancing of

applications of AI technology is certainly the case in Raman and surface-enhanced Raman spectroscopy (SERS) techniques, which involve large databases of complex vibrational spectra. Applying chemometric and analysis methods using manual techniques is no longer satisfactory for biomedical or diagnostic work. To implement accurate and powerful data analysis for Raman and SERS experiments, AI systems have recently been explored and implemented. A 2020 review article delves into the current uses of AI or machine (deep) learning techniques employed in Raman spectroscopy, including SERS (12).

An AI approach was applied to classify biomedical samples using Raman spectroscopy for the purposes of medical diagnosis and decision-making (13). The functional aspects of the AI system included automation of noise filtering (via a fuzzy controller), fluorescence background identification and correction, baseline optimization (using genetic algorithms), spectral normalization and scattering compensation (using the standard normal variate [SNV] algorithm), multivariate statistical analysis, sample data clustering, and projected decision-making. The AI program useful for classification of biomedical samples includes integration of fuzzy control, genetic algorithms, and principal component analysis (PCA), as well as system identification. The main goal for implementing the AI system is to incorporate a Raman probe on the end effectors of medical robots, to provide real-time information during robotic surgery.

A review paper, written in 2022, summarizes the application of Raman spectroscopy for noninvasive identification of mixture composition, including spectral preprocessing, and a detailed discussion of the application of AI analysis in Raman methods (14).

A 2022 research paper discusses the use of ML in FT-Raman spectroscopy for trademark fingerprint assessment of fruit spirits (15). The combination of ML and Raman spectra was used in an attempt to compose reliable models for the classification of fruit spirits for trademark, geographical, and botanical origin. Raman spectroscopy is an excellent measurement technique for samples with high water content, such as alcoholic beverages, due to the relatively weak Raman water bending mode in the fingerprint region. The discriminant analysis for the optimized classification model was reported to be 96.2% accurate. Geographical origin prediction was also achieved, but classification of botanical origin recognition was not successful. It was noted that spectral data used for the discriminant models involved both Stokes and anti-Stokes spectra, as well as individual spectral regions (windows). Several ML algorithm approaches were attempted. The paper offers an excellent discussion of the aspects of ML and Raman.

Raman spectroscopy provides an analytical method for non-destructively measuring the molecular structure for biomedical samples. Because of these benefits, Raman provides a suitable analytical technique for the assessment of inflammatory skin diseases and skin inflammation. The combination of AI with Raman spectroscopy to predict skin inflammation with high sensitivity and specificity was tested (16). For this feasibility work, Raman spectra, using excitation at 785 nm, were collected on mouse ear tissue where inflammation had been chemically induced. Principal component analysis (PCA) and AI were evaluated using receiver operating characteristic (ROC) curves to assess inflammation. The accuracy rate without AI implementation was 80.0% with an area under the curve (AUC) of 0.864. With AI implementation added, the accuracy rate was improved to 93.1% with an AUC of 0.972. The current findings demonstrate AI and Raman are able to provide highly accurate information on the presence and pathology of skin inflammation.

Raman spectroscopy has become known for its speed of analysis, limited requirements for sample preparation, ability to measure samples with high water content, and cost effectiveness. With these features, Raman is quite suitable for analysis of foods and beverages, and has been studied relative to classification and authenticity of such products. In one study, vegetable cold-pressed oils, which are of interest for nutritional health benefits, were tested for authentication analysis (17). In this study, oils from sesame, hemp, walnut, linseed, pumpkin, and sea buckthorn were tested for authentication using Raman spectra combined with ML. By using Raman spectra and ML, both adulteration and the degree of adulteration were successfully detected.

Improvements in chemometrics and data analysis techniques for Raman spectroscopy have allowed Raman to be used in more applications than ever before. However, there are still important issues to overcome when applying Raman spectroscopy that still limit its ability to fulfill its full analytical potential. These limitations include standardization of large datasets, intensity and baseline correction, fluorescence interference, measurement noise, changes in spectra relative to sample presentation variation, and so forth. In order to improve the quality and repeatability of Raman spectra, deep learning has been implemented as a strategy for enhanced correction of Raman spectral measurements. A book chapter devoted to these issues has been published with discussions, illustrations, and proposed solutions (18).

AI in Infrared (FT-IR) Spectroscopy

Gasoline quality prediction was tested using analytical data from gas chromatography (GC) and FT-IR on 45 gasoline samples (19). The AI system approach included preprocessing

implementation of principal component analysis (PCA) and fuzzy C means (FCM) algorithms. The FT-IR spectra were compressed and denoised using a discrete wavelet analysis method. The preprocessed data were analyzed using a hybrid neural network and support vector machines (SVM) classifier. The authors report an approximately 100% correct classification for six different categories of the gasoline using this workflow.

Lubricant oil efficiency is essential for maintenance of lubricated surfaces. The presence of water, aging (oxidation and decomposition), and contaminants can all seriously affect tribological (friction, wear, and lubrication) efficiency of oils. When oil efficiency is lost, longevity of metal parts and maintenance costs are a concern. In recent research, attenuated total reflectance (ATR) and Fourier transform infrared spectroscopy (FT-IR) were combined with AI techniques to assess lubricant oil status (20). The AI method consisted of using artificial neural networks (ANNs) with linear discriminant analysis (LDA) to derive analysis models for lubricant oils for the presence of water, as well as oil age and viscosity. The reported success for identifying the degree of oil deterioration was approximately 100% for the parameter of weeks of aging, and 97.7% for the parameters of viscosity and the presence of water.

Cereal quality is important for global human nutrition. The use of IR spectroscopy, hyperspectral imaging (HSI), and AI provides opportunities for quality monitoring of food and agricultural products. The combination of IR and HSI with AI provides high potential for improved measurements of food quality. A review article of these topics is given that describes the technical background, instrumentation, and data processing (preprocessing, feature extraction, and modeling) using AI approaches (21). The principles, advantages, challenges and future trends of IR and HSI integrated with AI are explored in this review.

FT-IR spectroscopy, in its traditional implementation, has shown great potential for food analysis applications—it is fast, non-destructive (noninvasive), and is capable of yielding a large quantity of chemical information. Recent successful applications include determination of spoilage in meat and the presence of microbial growth. For over two decades, ML has been used in combination with FT-IR to detect meat quality (22). In basic research, chicken breasts were purchased from a national retailer, comminuted for 10 s, and left to spoil at room temperature for 24 h. Every hour, ATR-FT-IR measurements were taken from the meat surface using the ATR technique. The IR spectral data were compared to total viable microbial counts determined using classical microbiology plating methods. The ATR-FT-IR spectra were processed using partial least squares (PLS) and genetic programming to provide accurate estimation

of bacterial loads within 60 s. The genetic programming was used to predict bacterial counts (bacteria/g) and onset of proteolysis (spoilage).

AI in Near-infrared Spectroscopy

Near-infrared (NIR) spectroscopy has had a long and established history of involvement with the fields of computer automation, computer networking, discriminant analysis, regression methods, spectral preprocessing, and ML in the form of neural networks (ANN and CNN). The field of chemometrics in spectroscopy was largely developed using NIR. In the late 1970s, all-possible-combinations (APC) search algorithms were in practice for optimizing multiple linear regression (MLR) calibration models. These APC models and techniques were referred to by Tomas B. Hirschfeld as "artificial intelligence" techniques, more or less—we would now refer to these as automated calibration programs. APC was capable of determining the optimized equation without additional human intervention. NIR techniques then progressed to the routine application of principal components regression (PCR), PLS, and ANN for quantitative calibrations and for classification problems. With this multi-decade experience in chemometrics, NIR applications have proliferated into many areas of commercial and research applications (23). Here, we give a few examples.

One study using NIR spectroscopy has applied AI DL to spectral analysis for cereal product composition measurements (24). For this research, NIR spectra were extracted using a deep learning-stacked sparse autoencoder (SSAE) method, with the prediction model constructed using an affine transformation (AT) and an extreme learning machine (ELM) algorithm. The authors report improved performance as compared to other classical (non-AI) NIR analysis calibration methods.

NIR spectroscopy is a prolific analytical technique applied for quantitative and qualitative analysis in the pharmaceutical, food, agricultural, materials, petrochemical, medical, and environmental sectors (23). The subject of mathematical preprocessing of NIR spectra prior to the modeling step has been addressed in many papers and books, and is an essential step in optimizing calibration models. Preprocessing steps can minimize the effects of particle size (for solids) and scattering (for liquids), as well as reduce spurious noise effects—all of which improve the performance of qualitative and quantitative calibrations.

A published paper describes the reduction of spectral noise using extreme learning machines, an approach which has demonstrated improvements in regression models and in large dataset classification work (25). This research reported the use of a parallel layer extreme learning machine (PL-ELM)

algorithm, and constrained (C)- PL-ELM, which has an architecture based on a non-linear layer in parallel with another non-linear layer. The details of this algorithm structure are explained within the paper. The method was tested on six real-life datasets, and the results for both regression and classification problems indicated that the root mean square error (RMSE) and accuracy were improved by applying this technique.

NIR has been used in the brewing industry over the years for analysis of raw ingredients and finished beverages. The analysis of beer faults early in the fermentation process can improve final product quality and consumer acceptance. In one study, AI was integrated with NIR spectra and the signal from an electronic nose (e-nose) (26). For this work, a commercial beer was spiked with 18 common beer faults plus the control aroma. The 19 aroma profiles were tested for classification analysis using an ML model. In total, six different ML models were developed. A Bayesian regularization algorithm was selected as the optimum method with model classification performance ranging from 95.3% to 98.9% accuracy without statistical signs of under- or overfitting.

AI in UV-vis Spectroscopy

Ultraviolet-visible (UV-vis) spectroscopy is widely recognized as a workhorse for general analytical laboratory, process, and field measurements. Water quality monitoring is just one of the many applications where UV-vis exhibits its beneficial features, such as speed, environmental friendliness, non-destructive sample handling, and high analytical sensitivity.

Water quality measurements using UV-vis for process or field applications have been quite common over the years. The application of ML to UV-vis spectroscopy provides an automated and “smart” platform for routine water analysis and screening (27). In this work, ML in the form of ANNs has been evaluated for simplifying water quality monitoring using UV–vis. Field water samples were collected, and spectra measured from 200 to 800 nm in a laboratory setting. Optimized CNN and PLS models were compared for water parameters resulting in an R^2 for total organic carbon (TOC) between predicted values and reference values to be 0.927 for PLS and 0.953 for the CNN model. Also, R^2 between predicted values and true values for total suspended solids (TSS) concentrations was 0.827 with the PLS model and 0.915 with the CNN model. It was concluded that CNN would be the preferred approach as compared to PLS for online water quality monitoring using UV–vis spectroscopy.

AI is being integrated with quantum chemistry and statistical mechanics for spectroscopic studies. One paper discusses the investigation of medium-to-large size chromophores in

condensed phases using UV-vis spectroscopy (28), where a prototypical nitroxide radical (TEMPO) was evaluated in different solvents. The paper explores the reliability, effectiveness, and robustness of the new AI platform for application to complex UV-vis spectroscopic studies.

Summary

From our brief survey of a few applications of AI to spectroscopic studies, we are able to discern that this advancing field will continue to change the development and capabilities of spectroscopic data analysis and implementation well into the future. AI has great positive potential when used properly with expert domain knowledge, and also great potential for misuse when blindly applied or when input data is inadequate or not well understood. Possibly we will be able to write future columns on this fascinating and rapidly emerging topic—we invite your feedback about this subject.

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