

Review Of Near Infrared Spectrum Detection Based on Deep Learning

Jingrui Liu *

University of Cincinnati Union College of Chongqing University Chongqing University, Chongqing, China

* Corresponding Author Email: sxscsa@gmail.com

Abstract. Near infrared spectroscopy technology has the characteristics of accurate analysis of material composition and characteristics, quantitative testing, non-destructive testing, and so on. With the progress of artificial intelligence and the development of deep learning technology, near-infrared spectroscopy detection systems based on deep learning algorithms have emerged, which include various typical methods and have achieved good application results in food safety monitoring, pollutant detection, and drug analysis. This article provides a systematic review of domestic and foreign literature, introducing the principles, characteristics, and development history of deep learning and near-infrared spectroscopy technology. It discusses the research significance of near-infrared spectroscopy detection based on deep learning. It also reviews the latest progress in deep learning based near-infrared spectroscopy related technologies, elaborates on the advantages, disadvantages, and applicable fields of the methods, and makes prospects and predictions for the future development trends in this field.

Keywords: Artificial Intelligence, Deep Learning, Near Infrared Spectroscopy.

1. Introduction

Near infrared spectroscopy (NIRS) is a technology that uses the near-infrared reflected light to detect the composition of substances. It has a series of advantages, such as fast detection speed, simple operation, non-destructive detection and so on. It is widely used in the fields of material analysis, medical diagnosis, food safety monitoring and biomedical research.

Compared with other spectral detection technologies, near infrared spectroscopy has its unique advantages. For example, it has unique recognition ability for organic substances and can realize non-invasive online detection. In addition, NIR spectroscopy can also realize nondestructive testing and sample analysis and can accurately distinguish unknown samples from real samples.

With the in-depth research and application of deep learning algorithm in computer vision and other fields in recent years, the research of using deep learning to process near-infrared spectral data and extract feature parameters has become a hot research direction. However, there are still many problems to be solved in the near infrared spectral image classification by deep learning: (1) The near infrared spectral data is large and high-dimensional; (2) In feature extraction, there are many parameters in the model network. Therefore, the research on deep learning and near infrared spectroscopy is necessary, which is also a topic worthy of further study in the future.

2. Overview of deep learning and near infrared spectroscopy

2.1. Development of deep learning technology

Deep learning is a branch of artificial intelligence that combines learning with artificial intelligence. This method is based on deep neural networks and continuously processes input data through deep learning to obtain new knowledge, thereby achieving higher levels of learning. Deep learning, which obtains knowledge from experience, can replace the step of formalizing tasks by humans. The concept of hierarchy allows computers to steadily transition from simple concepts to complex ones. If we draw a conceptual system diagram representing a task, we will obtain a "deep" (with many levels) graph, so this method is called deep learning [1,2].

The development of deep learning mainly has three stages: the first stage is the Back Propagation (BP) algorithm proposed by Rumelhart et al. [3] in the 1980s, which made the research of neural networks a reality, marking the embryonic stage of deep learning. However, the BP neural network was subsequently discovered to have gradient vanishing, leading most researchers to shift their focus from deep learning to shallow learning. The second stage was in 2006 when Professor Hinton [4] and his team applied a layer-by-layer initialization method to directly train the neural network, completely solving the gradient vanishing problem that exists in BP neural networks. At this point, deep learning has entered a stage of rapid development. The third stage was the first application of deep learning in the ImageNet image recognition competition in 2012, and in 2016, the AlphaGo program based on deep learning algorithm defeated the Go world champion Lee Sedol, promoting the rapid development of research results related to deep learning.

Compared with shallow learning, which lacks depth and is slow to train, deep learning methods can achieve fast, efficient, and accurate recognition of target objects, thereby improving recognition rate and accuracy. Figures 1 and 2 show the most representative network structure diagrams of two different algorithm models.

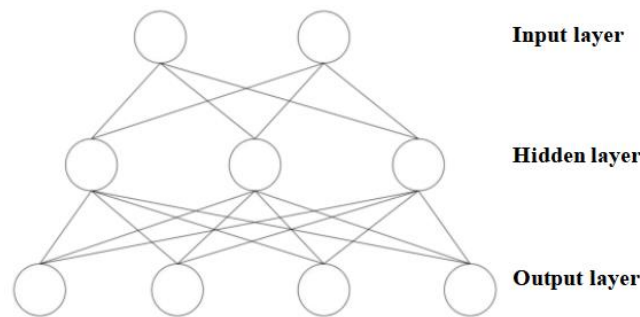


Figure 1. Structure diagram of shallow learning network

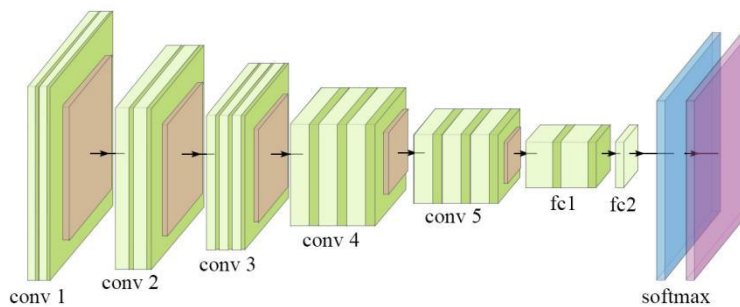


Figure 2. Structure diagram of deep learning network

At present, many deep neural network models, such as convolutional neural network (CNN), recurrent neural network (RNN) and short-term memory network (LSTM), have been widely used in the fields of pattern recognition, image processing and computer vision. Among them, convolutional neural network (CNN) and recurrent neural network (RNN) minimize the error between the network output and the pre-specified expected output (i.e., the clear label in the training set) through supervised learning [5]. The two methods have good effects in near-infrared spectral image classification, but their accuracy is still low, and overfitting is easy to occur in case of insufficient data. Long term and short-term memory network (LSTM) have a special memory cell structure and performs well in processing long sequences [6]. However, because it needs to input all data for memory storage, it cannot meet the requirements of near-infrared image classification.

2.2. Development of near-infrared spectroscopy related technologies

According to the wavelength range, the spectrum is usually divided into narrowband or broadband data, and the characteristic wavelength of near-infrared spectrum is 700-2500 nm. Near infrared spectroscopy (NIR) detection refers to the use of a spectrometer to collect the near-infrared radiation of a target substance. Based on the differences in absorption or emission spectra of the measured substance, quantitative correction methods are used to correct the measured spectrum, further completing the composition analysis and quality control of the sample and establishing a prediction model.

In 1800, British physicist F.W. Herschel discovered the near-infrared region of the spectrum. In the 1930s, near-infrared spectroscopy was mainly used to analyze and determine the chemical bond with high energy (such as CH, OH, NH, etc.) in various organic molecular structures. In the 1950s and 1980s, American professor Karl Norris compared a large number of measurement methods such as near-infrared transmission, reflection, and transmittance to obtain the reflection and absorption spectra of grains, and ultimately developed the first near-infrared spectrometer. Based on his research achievements, the US Department of Agriculture established the Near Infrared Spectroscopy Forage Research Center in 1978, sparking a small wave of near-infrared spectroscopy applications [7]. Since the 1980s, the rapid progress of computer science and chemometrics has provided a strong support for the development of NIRS technology. It has been used to detect water, protein, fat, starch in agricultural and sideline products, as well as different types of nutrients and trace elements in plants, which has achieved outstanding achievements. As we approached the 21st century, near infrared spectrum sensor (NIRS) was widely used in various agriculture, chemical industry, food industry and pharmaceutical industry.

3. Research status of near-infrared spectroscopy technology based on deep learning

3.1. Time distribution and literature quantity analysis

Conduct literature search in the CNKI citation database using the core keywords of "deep learning" and "near-infrared spectroscopy technology NIR\NIRS" (as of January 19, 2023, the search scope covers all literature from 2000 onwards). The results displayed that after excluding all irrelevant citation information, a total of 1669 relevant literature were found. By statistically analyzing and summarizing the results of relevant search papers (as shown in Figure 3), it can be clearly observed that after several consecutive years of steady and rapid increase in the number of relevant literatures from the end of 2004 to 2009, there was a slight fluctuation from 2009 to 2018. After the start of 2018, there was another blowout in relevant search papers, which continued until 2021. From the trend, the number of literatures will continue to rise after 2023, and at a certain time point, there may be another blowout period. From this, it can be seen that in the first decade of this century, the near-infrared spectroscopy detection technology and related applications based on deep learning achieved a qualitative change from quantitative change, achieving the first breakthrough. In the past five years, with the rapid development of artificial intelligence, deep neural networks, and gas detection technology, as well as the strong promotion of the government, related technologies and applications have gradually matured and shown a steady growth trend.

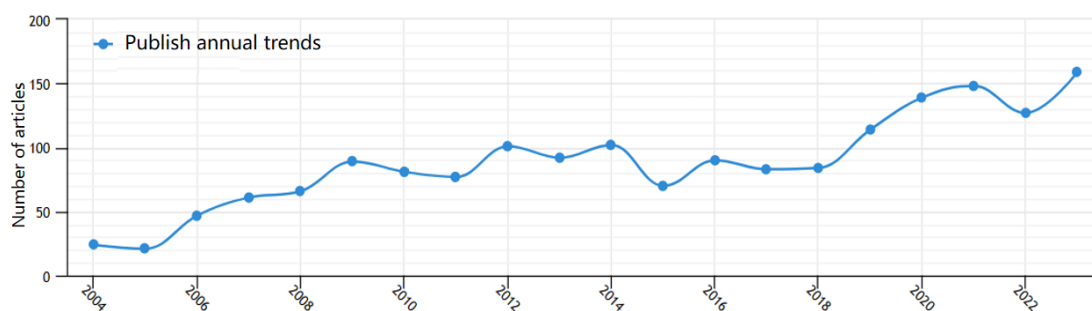


Figure 3. Trends in the publications in the near-infrared spectroscopy based on deep learning in the 20th century.

3.2. Applications

In recent years, deep learning based near-infrared spectral image classification algorithms have been widely applied in various fields. The algorithm flow chart is shown in Figure 4. First, the data set is trained by collecting samples, matching network structure, error function, etc., and then the relationship model between spectral features and target features is identified by deep learning to achieve food or environment detection. Three main advantages of it are listed compared with traditional chemometrics:

- (1) It has strong feature extraction capabilities, including super-resolution reconstruction, convolutional neural networks, etc;
- (2) It is capable of achieving sparse representation of near-infrared spectral data.
- (3) It improves the adaptability and robustness of the algorithm in complex spectral environments.

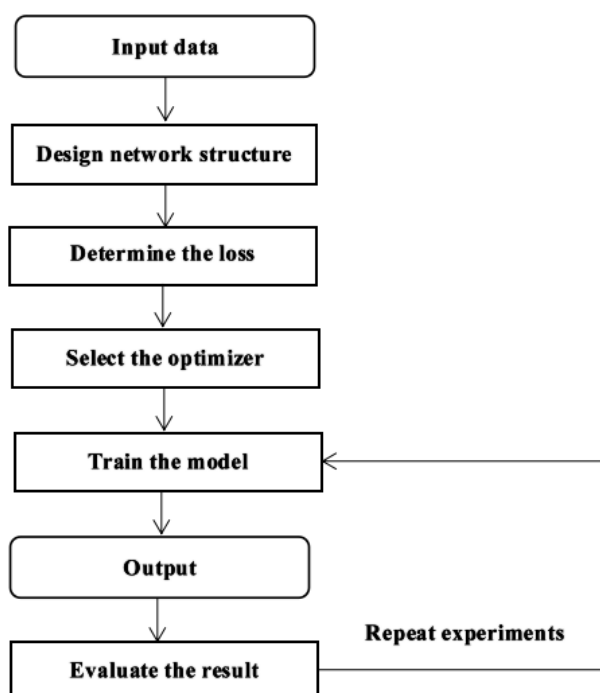


Figure 4. Flow chart of near-infrared spectroscopy algorithm based on deep learning.

Domestic and foreign scholars have conducted research on deep learning based near-infrared spectroscopy detection. In the field of agriculture, Vasseur Francois et al. [12] and Frontiers Production Office [13] identified the impact of growth conditions on trait values through deep learning of NIRS, which can capture a series of ecological information about plant diversity and function and accelerate the creation of a wide range of trait databases. There is also a DBN based tobacco quality classification model established by Wang Jing et al. [14], Peng Fa et al. [15]'s research

on fruit sugar content, and Wang Rujing et al. [16] and Liu Lanjun et al. [17]'s research on soil nutrients.

In the field of food safety, by combining traditional methods with deep learning algorithms, fast and accurate detection of target samples can be achieved. M N Australia et al. [18] used near-infrared spectroscopy and deep learning methods to predict macronutrients such as carbohydrates, proteins, lipids, etc. in infant food. Tang Hao [19] proposed a deep learning Li Net network that combines the generative adversarial network WGAN-GP and CNN-based SAE to address food safety issues in China and proposed an STL-XGBoost infant formula risk level warning method based on Time Series Decomposition (STL).

In the field of medicine and pharmacy, Li Ying et al. [20] focused on studying the predictive effect of blood glucose spectral concentration. Through OGTT experiments, near-infrared spectra and corresponding blood glucose concentration data in the fingertip region were collected, and support vector machine regression algorithm was used to predict blood glucose concentration. The articles by Xu Yajing et al. [21] and Zhang Weidong et al. [22] also focused on how to apply the NIRS method to drug feature recognition, in order to effectively solve many important theoretical problems encountered in clinical practice, such as fine classification of multiple subcategories, high-precision regression, model transfer, etc., reducing the design and training steps of simplified models, setting training parameters, and shortening training time. Fu Weifeng et al. [23] further optimized and improved the performance of the algorithm made by the system, taking the deep belief network method as the feature extractor and the random forest method as the spectral feature classifier, improving and improving the theoretical and application analysis processing capacity of the deep learning network algorithm under special conditions with relatively high requirements for the characteristic dimension of spectral data.

In the field of mining, Ba Tuan Le et al. [24] proposed a fast detection method for total aromatic hydrocarbon content in diesel based on deep learning algorithms and near-infrared spectroscopy. LE Ba Tuan et al. [25] established a model for coal mine spectral classification by comprehensively applying deep learning, extreme learning machine ELM algorithm, and infrared spectroscopy. They found that compared with traditional and cumbersome manual methods and chemical analysis methods, CNN network algorithm can capture more details of spectral features, and combined with ELM classification model, it has relatively good classification performance, and has unparalleled advantages in economy, speed, and accuracy.

In the field of electronic information, deep learning based near-infrared spectroscopy detection is mainly used for image recognition and processing. For example, Lv Shangjin [26] constructed an RGB-NIR image dataset and proposed an AEDNet network model for color restoration of RGB-NIR images under low illumination, achieving satisfactory results. Mei Shaohui et al. [27] established a residual learning based infrared spectral band image prediction analysis and processing network by combining the near-infrared spectral band configuration of the AVIRIS imaging spectrometer. They used computational imaging to predict spectral images in the near-infrared band from hyperspectral images in the visible light range, effectively improving the accuracy of hyperspectral data processing and providing new technical support for capturing images in single photosensitive chip imaging systems.

The above studies have shown that deep neural networks can learn key features from the original spectrum, greatly reducing the difficulty of feature extraction. The combination of multiple processing layers improves fitting and feature extraction capabilities, making it suitable for various analysis tasks. Advanced deep learning architecture and embedded regularization technology significantly reduce the risk of over fitting [28]. However, the construction of the model requires a large amount of data training, which is a time-consuming and lengthy process. At present, most deep learning models are only applied in certain specific fields and cannot be generalized in other fields. With the advent of the big data era, people are increasingly using different types of data for modeling work, thus placing higher demands on model algorithms.

4. Outlook and prediction of development trends

Currently, deep learning based near-infrared spectroscopy detection methods have gradually matured and improved. The development of near-infrared spectroscopy technology in China started relatively late, but it has been relatively rapid. In the mid-1990s, many domestic research institutes began actively researching and developing complete sets of analytical techniques suitable for domestic needs and did a lot of work for the popularization of this technology, creating a new situation for NIR research and application in China [29]. The first National NIR Spectroscopy Academic Conference in 2006 and the NIR Spectroscopy Professional Committee established in 2009 have played a major role in helping the development of domestic NIR spectroscopy technology. In the past decade, many algorithms based on convolutional neural networks have been proposed and applied to near-infrared spectral detection. However, due to the large amount of interference factors, nonlinear information, unstructured information, complex correlation relationships, and large datasets in complex spectral data such as food, the use of convolutional neural networks for near-infrared spectral detection and prediction faces difficulties and challenges. In addition, in practical applications, due to the small sample dataset and large number of variables, traditional convolutional neural network models are difficult to accurately predict these complex and ever-changing situations. The author thinks that in the future, near-infrared spectroscopy detection systems based on deep learning algorithms will develop in three directions: (1) By introducing diverse datasets, model accuracy will be further improved; (2) By adding attention mechanism and loss function, we can make full use of multi-layer network structure and data set characteristics to elevate the algorithm performance; (3) The instrument will achieve further lightness and portability, while reducing price and improving accuracy.

5. Conclusion

This article summarizes the research background and technical principles of deep learning based near-infrared spectroscopy detection through literature research and summarizes the cutting-edge applications and research status of this method in various fields. Through comparative analysis, this method is compared with traditional methods such as shallow learning and chemical analysis to clarify the advantages and research shortcomings of the new method. The advantages of deep learning based near-infrared spectroscopy detection are fast detection speed, simple operation, non-destructive, and wide application fields. However, its large data volume, high-dimensional data, and multiple model parameters may consume a lot of time and resources during the training process. Moreover, the existing small models only focus on a specific field and do not have a universal large model, posing higher requirements for model algorithms. Finally, this article predicts the future development trends in this field, mainly through big data, deep learning to improve model accuracy, algorithm performance, and instrument lightness, in order to better adapt to the requirements of application scenarios.

References

- [1] Goodfellow I, Bengio Y, Courville A. Deep learning[M]. Massachusetts: MIT press, 2016. 8-16.
- [2] Feng Xin. Research and Implementation of Pedestrian Attribute Recognition Technology Based on Semantic Segmentation [D], 2019.
- [3] Rumelhart D.E., Hinton G.E., Williams R.J. Learning internal representation by back-propagation of errors [J]. Nature,1986,323(323):533~536.
- [4] Hinton G.E., Osinero S., Teh Y. A Fast-Learning Algorithm for Deep Belief Nets [J]. Neural Computation,2006,18(7):1527.
- [5] Zhu Youzhuo, Liu Hongyu, You Yuhao, Zheng Heng. Progress in the application of deep learning in the study of antimicrobial peptides [J]. Chinese Journal of Antibiotics, 2023,48 (04): 374-380.

- [6] Hua Fan, Li Li, Cai Xinnan, Xu Jian. Application of short-term memory network in temperature prediction [J]. *Intelligent Computer and Application*, 2022,12 (11): 92-95+102.
- [7] Norris K. History of NIR [J]. *Journal of Near Infrared Spectroscopy*, 1996, 4(1): 31-37.
- [8] Vasseur François, Cornet Denis, Beurier Grégory, Messier Julie, Rouan Lauriane, Bresson Justine, Ecartot Martin, Stahl Mark, Heumos Simon, Gérard Marianne Reijnen Hans, Tillard Pascal, Lacombe Benoît, Emanuel Amélie, Floret Justine, Estarague Aurélien, Przybylska Stefania, Sartori Kevin, Gillespie Lauren M., Baron Etienne, Kazakou Elena, Vile Denis, Violle Cyrille. A Perspective on Plant Phenomics: Coupling Deep Learning and Near-Infrared Spectroscopy [J]. *Frontiers in Plant Science*,2022,13(13).
- [9] Frontiers Production Office. Erratum: A perspective on plant phenomics: Coupling deep learning and near-infrared spectroscopy [J]. *Frontiers in Plant Science*,2022, 13(13).
- [10] Wang Jing, Dingxiangqian, Wang Xiaodong, Han Feng, Han Dong, Qu Xiaona. Research on Near Infrared Spectral Classification of Tobacco Leaf Parts Based on Deep Belief Network [J]. *Infrared and Laser Engineering*, 2019,48 (04): 31-37.
- [11] Peng Fa, Wang Zhen, Liu Shuangxi, Wang Jinxing, Yang Huawei. Near infrared sugar content prediction based on partial least squares and deep learning [J]. *Journal of Jilin Agricultural University*, 2021,43 (02): 196-204.
- [12] Wang Rujing, Chen Tianjiao, Wang Yubing, Wang Liusan, Xie Chengjun, Zhang Jie, Li Rui, Chen Hongbo. A prediction model for soil near-infrared spectroscopy analysis based on deep sparse learning [J]. *Journal of Luminescence*, 2017,38 (01): 109-116.
- [13] Liu Lanjun, Zhai Yongqing, Zheng Junjun, Fan Pingping, Deng Li. Visible/near-infrared spectral modeling of soil nitrogen content based on deep learning [J]. *spectroscopy and Spectral Analysis*, 2020,40 (S1): 71-72.
- [14] M N Aulia, M L Khodra, A P Koesoema. Predicting Macronutrient of Baby Food using Near-infrared Spectroscopy and Deep Learning Approach [J]. *IOP Conference Series Materials Science and Engineering*, 2020, 803(1).
- [15] Tang Hao. Research on Typical Food Safety Risk Early Warning Based on Machine Learning [D], 2022.
- [16] Li Ying, Zhou Linhua. Research on non-invasive blood glucose concentration regression based on near-infrared spectroscopy and machine learning [J]. *Journal of Changchun University of Technology (Natural Science Edition)*, 2022,45 (03): 138-143.
- [17] Xu Yajing, Yu Jie, Yu Yuanpan, Li Xuefang, Li Jingping. Application of artificial intelligence in the identification of traditional Chinese medicine and decoction pieces [J]. *Chinese Journal of Traditional Chinese Medicine*, 2022,40 (08): 47-50.
- [18] Zhang Weidong, Li Lingqiao, Hu Jinqian, Feng Yanchun, Yin Lihui, Hu Changqin, Yang Huihua. Drug identification by near-infrared spectroscopy based on stack sparse self-coding fusion kernel limit learning machine [J]. *analytical chemistry*, 2018,46 (09): 1446-1454.
- [19] Fu Weifeng, Yang Huihua, Liu Zhenbing, Feng Yanchun. Drug identification methods based on deep belief network and random forest [J]. *Computer Simulation*, 2018,35 (04): 325-330.
- [20] Ba Tuan Le, Thai Thuy Lam Ha. Total aromatics of diesel fuels analysis by deep learning and near-infrared spectroscopy [J]. *Spectroscopy Letters*,2019,52(10).
- [21] LE Ba Tuan, Xiao Dong, Mao Yachun, Song Liang, He Dakuo, Liu Shanjun. Coal classification by visible and near-infrared spectroscopy and deep learning CNN-ELM algorithm [J]. *spectroscopy and Spectral Analysis*, 2018,38 (07): 2107-2112.
- [22] Lv Shangjin. Color Restoration of Near Infrared RGB Images under Low Illuminance Based on Deep Learning [D], 2022.
- [23] Mei Shaohui, Zhang Bowei, Ma Mingyang, Jia Sen. Near infrared hyperspectral image data prediction technology [J]. *Chinese Journal of Image Graphics*, 2021,26 (08): 1786-1795.
- [24] Xu Lingjie. Research on the Application of Deep Learning in Near Infrared Spectroscopy Analysis Technology [D], 2019.
- [25] Chu Xiaoli, Yuan Hongfu, Lu Wanzhen. Research and application development of near-infrared spectroscopy analysis technology in China in recent years [J]. *Analytical Instruments*, 2006 (2): 1-10.