CHEMICAL MINING USING BIG DATA IMAGE ANALYTICS WITH DEEP THREE-DIMENSIONAL CONVOLUTIONAL NEURAL NETWORK

A Ramana Lakshmi[a], Mudassir Khan[b], Ranichandra C[c], Papiya Mukherjee[d], Veeramalai Sankaradass[e], Madiajagan M[f]

Article History: **Received:** 10.09.2022 **Revised:** 15.10.2022 **Accepted:** 19.11.2022

Abstract: With intense competition that exists in the mining sector around the world, improvements in both product performance and energy economy are absolutely important. This presents a one-of-a-kind obstacle due to the fact that the demand for raw resources is constantly growing, despite the fact that vast supply of high-quality commodities are rapidly running out. The ability to correctly identify chemicals is a skill that is crucial to the investigation of a wide range of subjects. Conventional methods for determining the identity of chemicals take a significant amount of time and demand a substantial number of resources due to the fact that they impose a significant amount of reliance on the knowledge of the identifier as well as on external equipment. Technology based on deep learning has made it possible for people to identify chemicals in a way that requires significantly less time and effort, as well as a significant reduction in the number of errors produced.

Keywords: Chemical, Mining, Big Data, Three-Dimensional Convolutional Neural Network

[a]. Associate Professor, Department of CSE, Prasad V Potluri Siddhartha Institute of Technology, Vijayawada, Andhra Pradesh, India
[b]. Assistant Professor, Department of Computer Science, College of Science & Arts Tanumah, King Khalid University, Abha, Saudi Arabia.
[c]. Associate Professor, School of Information Technology and Engineering, Vellore Institute of Technology, Vellore, Tamil Nadu, India.
[d]. Assistant Professor, Koneru Lakshmaiah Education Foundation, Department of Computer Science and Engineering, Green Fields, Vaddeswaram, Guntur, Andhra Pradesh, India.
[e]. Professor, Department of Computer Science and Engineering, Chennai Institute of Technology, Chennai, Tamil Nadu, India.
[f]. Associate Professor, School of Computer Science and Engineering, Vellore Institute of Technology, Vellore, Tamil Nadu, India.

***Corresponding Author**

E-mail: arlakshmi@pvpsiddhartha.ac.in

DOI: 10.31838/ecb/2022.11.11.012

INTRODUCTION

In order to treat ore successfully from the mine to the mill and beyond, new methods need to be developed to describe the ore components and assess the ore prospective performance in applications farther down the processing chain [1]. Utilizing cutting-edge methods for liberation analysis and chemical characterization is necessary if one want to provide a more precise description of ore bodies and the subsequent processing of ore resources [2] [3].

Chemical-based technologies have a history of success, particularly in the fields of chemical identification and liberation analysis (MLA). The process of identifying chemicals provides a plethora of information, not only about the chemical composition of an ore but also about the textural properties of the ore. When planning comminution and leaching procedures for chemical processing, one of the most important steps is to make use of chemical liberation data [4].

In a number of investigations, in particular this one, the two-dimensional chemical layer analysis (MLA) and a matching two-dimensional slice derived from micro-CT data were compared and contrasted regarding chemical segmentation. On the other hand, past knowledge in the form of 2D MLA chemical data is not utilized in any way during the segmentation phase of the process. This is done so that the procedure can proceed more smoothly [5].

Complex algorithms [6]-[12] that make use of computer vision are required in order to tackle the issues that have been brought to light with 2D MLA and current 3D MLA operations. These issues have been brought to light as a result of recent research. One method that is believed to be on the cutting edge of computer vision is the use of a convolutional neural network (CNN) that has been trained in a deep learning framework. It has been put to extensive use in geoscientific contexts for the aim of semantic segmentation.

BACKGROUND

The process of anticipating and evaluating the geological chemical resources is broken down into several stages. One of these stages is called intelligent prospecting. The transition took place gradually in the recent years. This phase was brought

about as a result of this transition. With the goal of simplifying the process of trading huge datasets, a number of distinct big data cloud platforms have been established. Some examples of these platforms include cloud computing, data clouds, and automatic text reading. One aspect that helps to the advancement of the quantitative assessment of chemical resources is the availability of technologies that are capable of analyzing huge amounts of data [12]. This is just one of the factors [13], because digital geology in this age of big data stimulates the development of geological prospecting.

In addition, when evaluating and making use of big data in the field of geology, it is necessary to take into consideration the characteristics of geological data as well as the requirements of the geological field [14].

In addition, the methodology behind prospecting has been comprehensively summed up [15], with an emphasis on the usage of huge volumes of geological data [16]. These theories are as follows: chemical prediction model theory, chemical prediction correlation theory, trend analysis method, and differentiation theory. These theories are the trend analysis method, differentiation theory, chemical prediction model theory, and chemical prediction correlation theory.

The model in [17] has provided an innovative strategy that is driven by models in this day and age of big data science. In this approach, geological theory is used to determine how to interpret geological data, and computer technology is utilized to mine large amounts of geological data. The objective is to arrive at more precise forecasts on the times at which chemical resources will be available.

The metallogenic theory and prediction could be brought about by geological big data after providing a comprehensive summary of the use of geological big data in the study of metallogenic regularity, metallogenic series, and metallogenic systems. He came to this conclusion after providing a comprehensive summary of the use of geological big data in the study of geological big data. [18] As a result of this finding, due to his belief that the future information wealth could only be obtained by efficiently extracting information in accordance. He did this because he believed that this was the only way that the information wealth could be obtained in the future.

Big Data relies on the usage of extremely large amounts of data. If there is not a need that has been expressed clearly for the data or a method that is effective to mine the data, then the data will be meaningless. The idea of big data is not predictive in and of itself; rather, the process of moving from the known to the unknown may be labelled predictive thinking, and it entails mining data for probable knowledge. Predictive thinking requires shifting from the known to the unknown. The transition from the known to the unknown is an essential part of predictive thinking. In order to take chemical resource prediction to the next level of intellectualization, not only do we need to incorporate a wide range of data analysis algorithms, but we also need to set up a perfect and effective theoretical system of big data prediction methodologies. Only then will we be able to take chemical resource prediction to the next level of intellectualization. After that, and only then, will we be able to advance the amount of intellectualization achieved by our chemical resource projection.

PROPOSED METHOD

In this paper, not only is an intelligent prediction method that takes into account, the main focus, the prediction model, is successful. All of this is done with the goal of enhancing the efficacy and accuracy of the predictions produced on chemical resource availability.

In this manner, the algorithm gradually gets closer to the optimal combination and accomplishes the ore targets by automatically learning the logical principles and developing the mechanism of random combination of the ore-controlling components. The algorithm is able to accomplish its ore targets as a result of this. This method can be utilized to assist with a variety of tasks, including the mining of intelligent geographical data as well as the analysis of decisions.

The Chemical Liberation Analyzer and the QEMSCAN have swiftly become the most popular approaches in comparison to other semi-automated SEM and optical microscopy technologies. This is primarily attributable to the fact that they are substantially less costly and need a significantly lower amount of time to analyze. It is necessary to collect a significant amount of physical information from the MLA in order to develop effective ways for processing chemicals. This information should include details such as the size of the pieces, the quality of the chemicals, how they feel, and how much they release.

It is widely knowledge that sampling mistakes and stereological effects may occur whenever a two-dimensional analysis is performed on a three-dimensional fragment structure. Because of this, it is likely that such an analysis will not be adequate for completely defining the physical qualities of the ore samples that have been examined. A 2D mapping of a polished ore cross-section is generated for automated chemical liberation analyzers such as QEMSCAN, which can only identify the chemicals on the polished surface.

Any structural information received from the ore sample is pointless because it must first be ground into a powder before the XRD instrument can be used on it. The chemical composition of a complete sample can be determined using XRD measurements; however, these data do not provide any information regarding the location of the individual chemicals or the associations they have with one another. Because of its capacity to explore local information as well as calibrate with other methods, micro-XRD is a viable tool for 3D MLA. The micro-XRF and QEMSCAN methods are significantly faster than this one.

Recent developments have resulted in the creation of a novel technique known as high-resolution 3D X-ray microcomputed tomography (micro-CT), which aims to circumvent the shortcomings of traditional 2D imaging. The microscale structure of rocks may be analyzed with the use of this technology, which is non-invasive and non-destructive at the same time. Micro-CT has been applied in a number of research initiatives conducted by MLA in order to explore the three-dimensional fragment structure as well as the spatial groupings. In MLA, it is required to split images into classes, where each voxel represents a certain chemical or pore space. This is done using the MLA image classification system. The study that has been done utilizing micro-CT for MLA has been beset by a variety of methodological difficulties, despite the fact that this was a good beginning.

Due to the fact that the attenuation of an X-ray is correlated to the density of a chemical, micro-CT scans of a variety of chemicals that have comparable densities are unable to discern amongst one another. This is because the attenuation of an X-ray is proportional to the density of a chemical. In order to determine the chemicals that are present, standard segmentation algorithms often make use of the X-ray attenuation, also known as the value of each particular voxel. Neither the chemical structure nor the textural features were taken into consideration when carrying out the procedure of segmentation.

It is impossible to completely remove human bias from the segmentation process due to the fact that the criteria for doing so are specified by the user. Because of this, the determination of where fragment borders are located and, ultimately, the findings of the study are influenced. When it comes to segmentation, many research fail to take into consideration the cross-sectional data that might be supplied by 2D MLA. This is because 2D MLA requires multiple measurements.

3D CNN

In this part of the article, there is a stacked block convolutional neural network (SB-3D-CNN) that uses 3D convolution to combine spectral and spatial input together. The proposed methodology is broken down into three distinct stages. The first step is called dimensional reduction, and it uses principal component analysis (PCA) and neighbourhood extraction to cut down on the number of spectral and spatial dimensions as well as redundant information. This approach is able to maintain the spectral dimensions that are considered to be the most significant. The example of Indian Pines (IP) is used to explain the dimensions reduction aspect of the process. Based on the dimensions of the original data, which were 145×145×200, the input of the network is turned into patches have been performed on it.

In the subsequent stage, the procedure of feature extraction and filtering is carried out. During this stage, a five-block structure that includes an attention layer is utilised. Each block contains three-dimensional convolutional layers, each of which has a one-stride and a two-stride stride. The major contributions of this step are the extraction and compilation of abstract features, followed by the removal of information that interferes with the process. In order to achieve pooling layer downsampling. The data from the HSI tensor will not be protected by the proposed design because it does not use a pooling layer. Padding can be used to control the boundary effect, and while employing this method, the size of the output is maintained to be consistent with that of the input. The batch normalisation step that comes after each convolutional layer has the potential to speed up the convergence process even further.

After that, the spectral-spatial characteristics are categorised with the help of a fully linked layer. The softmax activation strategy is utilised in the categorising step. The output of the fully linked layer contains n different kinds of conditional probabilities. It is possible to utilise a formula.

$$P\left(Y=m\middle|X',k,r\right)=f\left(kX'+r\right)=\frac{e^{k_1X'+r_1}}{\sum_j e^{k_jX'+r_j}}$$

where k - weight value, m- belongs to a category and r - bias term.

The 3D-architecture is depicted here in Figure 1.

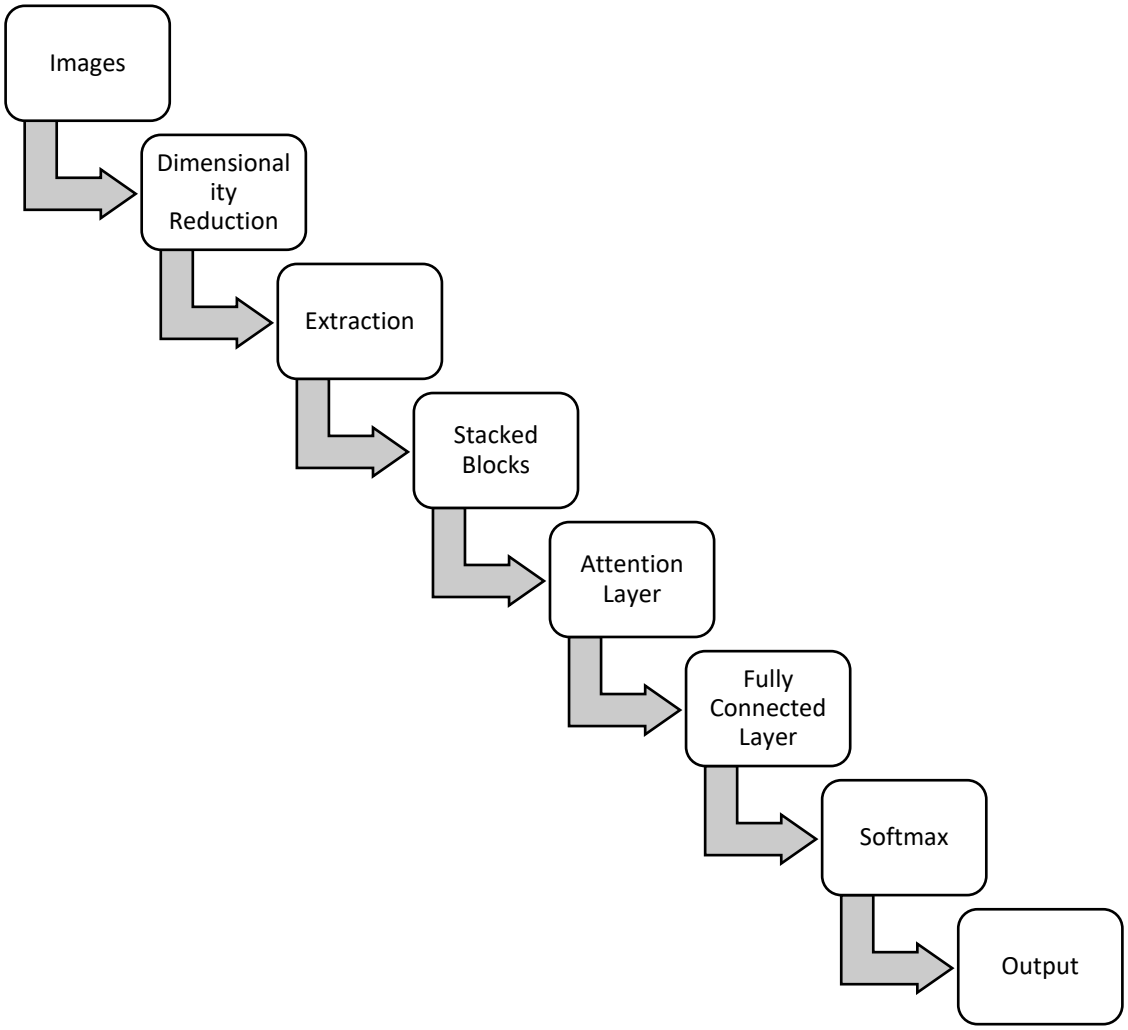

Figure 1: 3D-CNN

RESULTS AND DISCUSSIONS

The MinDat-Chemical-Image-Dataset repository on GitHub makes available for download an assortment of about half a million labelled photos of chemicals taken from mindat.org. The collection was created by loliverhennigh. The dataset is collected from GitHub - loliverhennigh/MinDat-Chemical-Image-Dataset: A dataset of +500,000 chemical images with labels taken from mindat.org.

In order to validate our neural network model, we selected 13,911 images out of a total of 220,057 photos to test. This allowed us to determine whether or not the model was successful. When one of the photos is loaded into the neural network, it will provide a classification of the chemicals that are most likely to be present in the image. In this part of the study, the accuracy of our approach is evaluated and compared to the accuracy of a number of different ways, and the findings of our inquiry are presented.

It is necessary to collect a massive amount of data in order to put YOLOv5 chemical identification training through its paces and validate its results. When a model has access to a greater quantity of training data, this leads to increases in the model accuracy, generalizability, and robustness. Mindat is the most extensive database of chemical information in the entire world, and it is handled cooperatively by a network of chemical experts from all around the world. As part of the preliminary work for the project, images of fifty different types of chemicals were gathered. One of the aspects that contributes to the limited availability of some chemicals is the rarity of the chemicals themselves. For instance, the rarity of certain chemicals makes it difficult to obtain an adequate number of samples. This is one of the factors. It is essential to make note of the fact that each and every chemical specimen has been accurately labelled and arranged in accordance with the criteria established by Mindat. It is possible that some of the photographs that were downloaded from the internet were altered in some manner, or that they were captured using a microscope. Both of these things could have an effect on the credibility of the findings. As a consequence of this, while we were compiling the data, we excluded from consideration the photographs that did not meet the prerequisites of the dataset based on our own arbitrary

criteria. First thing that we did was take all of the collected chemical photos and segregate them into three distinct sets: a training set, a validation set, and a test set. These sets were used for training, validating, and testing the classification system.

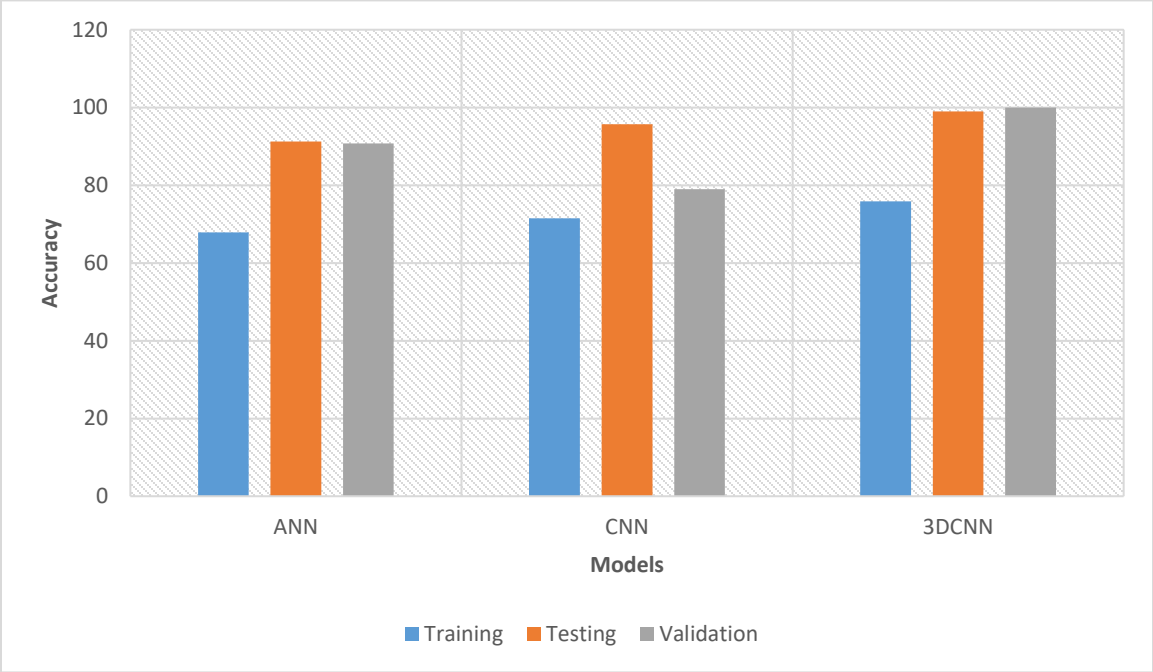

Figure 2: Accuracy

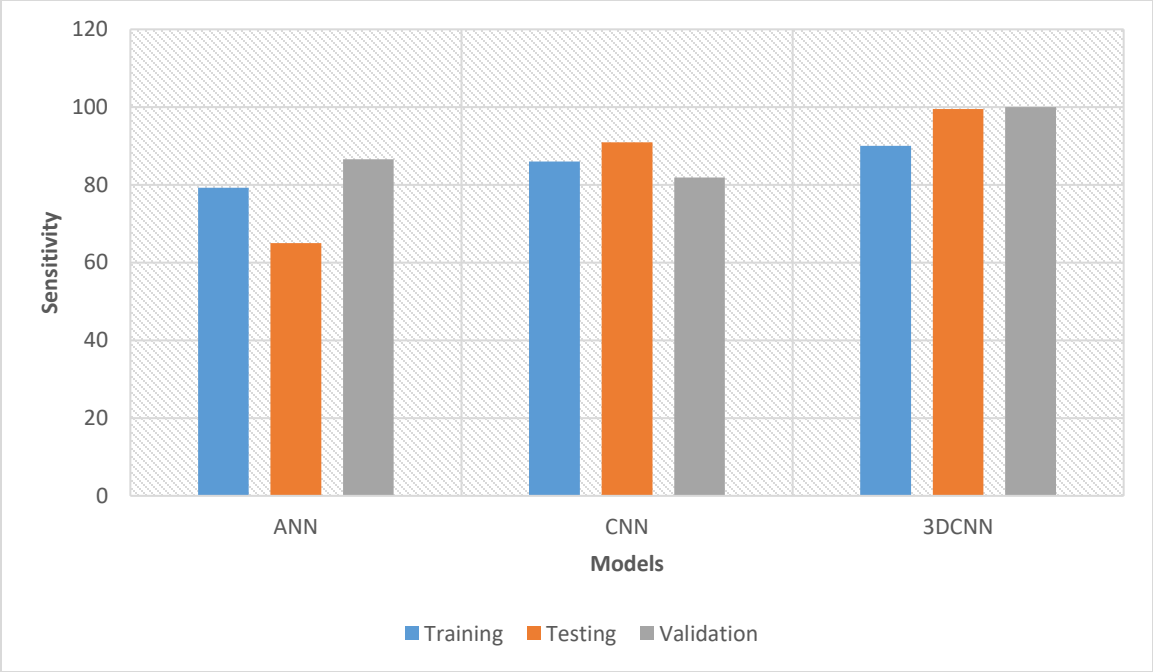

Figure 3: Sensitivity

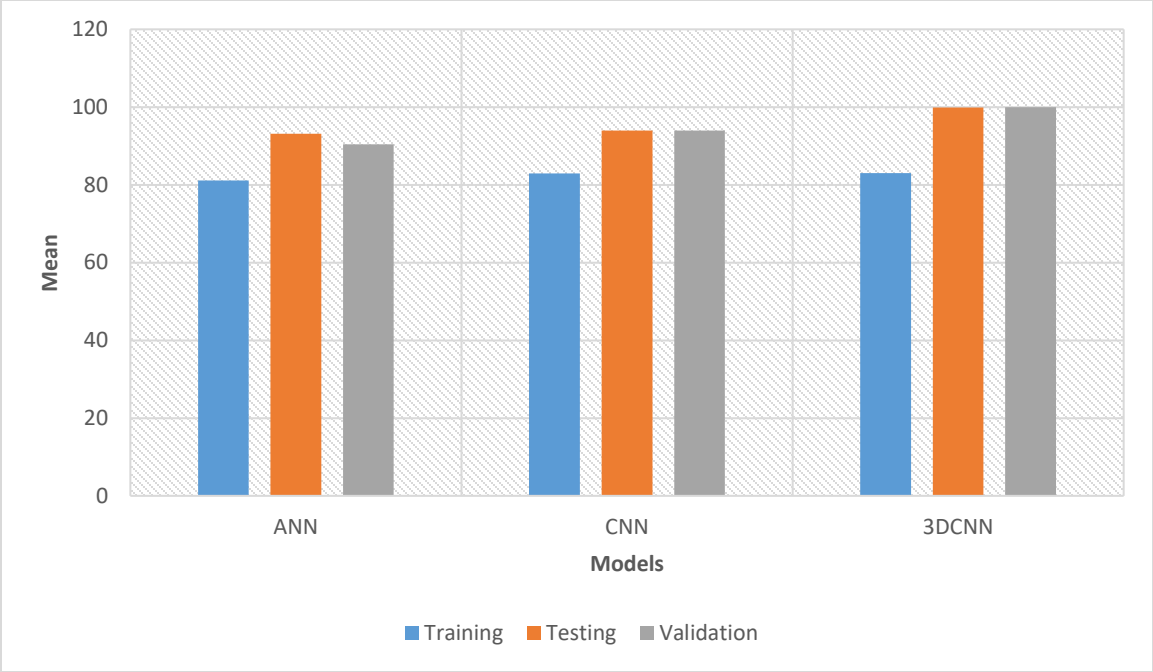

Figure 4: Mean

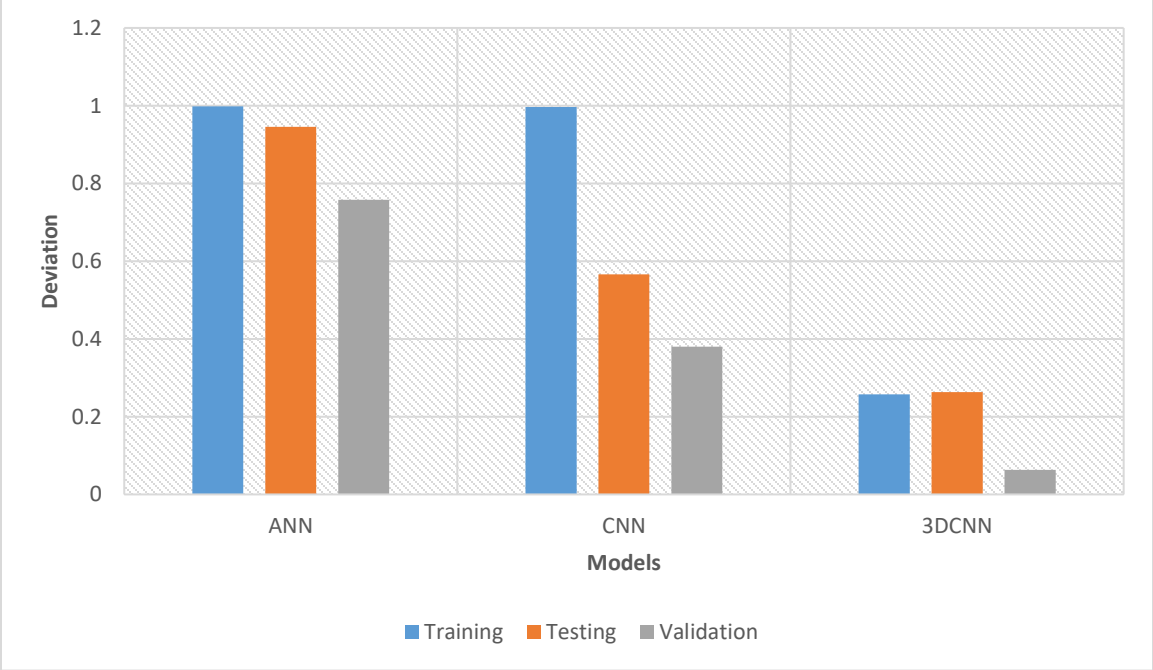

Figure 5: Standard Deviation

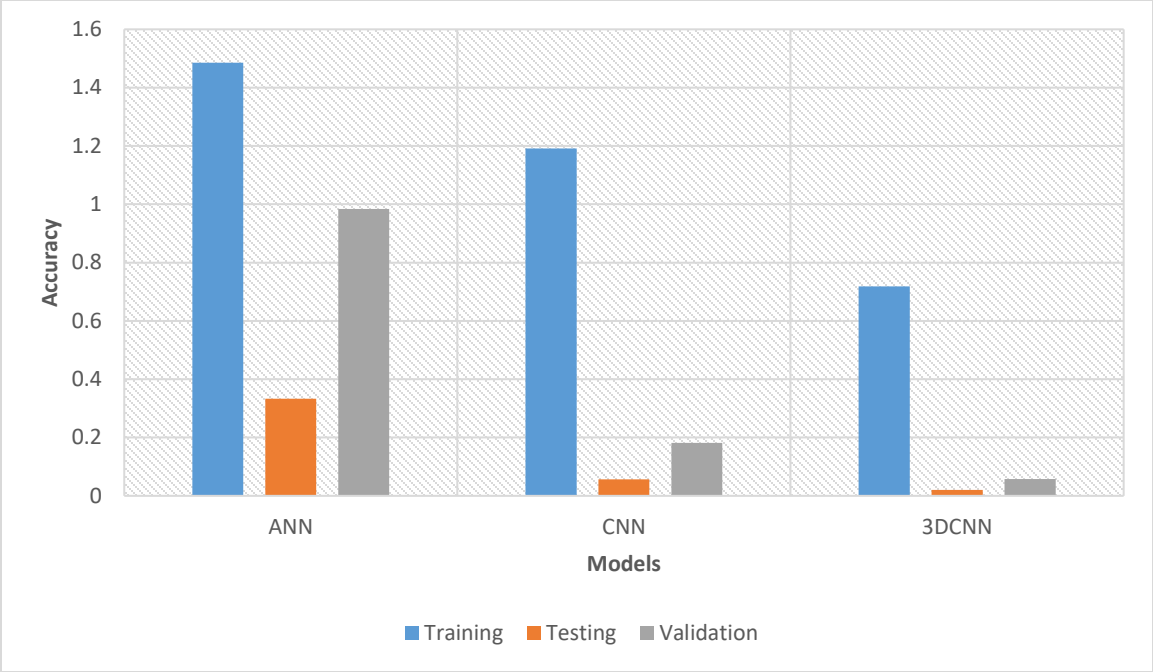

Figure 6: MAPE

Figure 2- 6 contains the findings of our experiments that made use of the 3D-CNN. When analyzing images with either an insufficient or an excessive quantity of light, the results that we acquired are presented in this table as an average accuracy. The findings of the trials indicate that improving identification precision by combining the Laplace and 3D-CNN algorithms in some way can greatly increase the accuracy of the process.

All of our chemicals have been correctly identified to a degree of accuracy that is at least 80%, with the exception of a few chemicals that are exceptionally uncommon in the general population. Four of these chemicals have poor precision since they did not acquire adequate training. The reason for this is as follows: In instance, the application of Laplace in conjunction with 3D-CNN resulted in a 10% increase in the precision of the chemical detection process. When compared to the conclusions that were obtained without the assistance of Laplace, this is an improvement.

The primary challenge is that many different chemicals have shapes and textures that are very similar to one another. This makes it challenging for the model to correctly identify the chemicals based on photographs that were taken in insufficient or extremely high light, which causes chromatic aberrations. Because of this, it is one of the components of the problem that is the most challenging. Because the chemicals are too dark and have less of an effect when exposed to light, using Laplace theory does not result in a considerable improvement in accuracy.

CONCLUSIONS

We present a deep learning approach to chemical detection that makes use of 3D-CNN as part of the scope of this work. We are able to significantly improve the accuracy rate of chemical identification in comparison to the algorithms that were traditionally used for chemical identification by lowering the impact that the intensity of the illumination has on the chemical identification process. We made use of 3D-CNN during the portion of the deep learning process that was devoted to recognition so that we could achieve an even higher level of accuracy. We employed the fine-tuned 3D-CNN to boost the identification precision even further, which we did when we were selecting models to use.

REFERENCES

i. Xu, Y., Liu, X., Cao, X., Huang, C., Liu, E., Qian, S., ... & Zhang, J. (2021). Artificial intelligence: A powerful paradigm for scientific research. The Innovation, 2(4), 100179.

ii. Morlock, G. E. (2021). High-performance thin-layer chromatography combined with effect-directed assays and high-resolution mass spectrometry as an emerging hyphenated technology: A tutorial review. Analytica Chimica Acta, 1180, 338644.

iii. Debus, B., Parastar, H., Harrington, P., & Kirsanov, D. (2021). Deep learning in analytical chemistry. TrAC Trends in Analytical Chemistry, 145, 116459.

iv. Debus, B., Parastar, H., Harrington, P., & Kirsanov, D. (2021). Deep learning in analytical chemistry. TrAC Trends in Analytical Chemistry, 145, 116459.

v. Giordano, G. F., Freitas, V. M., Schleder, G. R., Santhiago, M., Gobbi, A. L., & Lima, R. S. (2021). Bifunctional Metal Meshes Acting as a Semipermeable Membrane and Electrode for Sensitive Electrochemical Determination of Volatile Compounds. ACS Applied Materials & Interfaces, 13(30), 35914-35923.

vi. Yang, J., Li, J., Hu, J., Yang, W., Zhang, X., Xu, J., ... & Ying, Y. (2022). An interpretable deep learning approach for calibration transfer among multiple near-infrared instruments. Computers and Electronics in Agriculture, 192, 106584.

vii. Cadeado, A. N., Machado, C., Oliveira, G. C., Silva, D. A., Muñoz, R. A., & Silva, S. G. (2022). Internet of Things as a Tool for Sustainable Analytical Chemistry: A Review. Journal of the Brazilian Chemical Society, 33, 681-692.

viii. Schade, F., Schwack, W., Demirbas, Y., & Morlock, G. E. (2021). Open-source all-in-one LabToGo Office Chromatography. Analytica Chimica Acta, 1174, 338702.

ix. Tan, X., Liang, Y., Ye, Y., Liu, Z., Meng, J., & Li, F. (2022). Explainable Deep Learning-Assisted Fluorescence Discrimination for Aminoglycoside Antibiotic Identification. Analytical Chemistry, 94(2), 829-836.

x. Wang, X., Chen, S., Wu, M., Zheng, R., Liu, Z., Zhao, Z., & Duan, Y. (2021). Low-cost smartphone-based LIBS combined with deep learning image processing for accurate lithology recognition. Chemical Communications, 57(58), 7156-7159.

xi. Lee, S. M., Balakrishnan, H. K., Yuan, D., Nai, Y. H., & Guijt, R. M. (2021). Perspective-what constitutes a quality analytical paper: Microfluidics and Flow analysis. Talanta Open, 4, 100055.

xii. Amor, N., Noman, M. T., Petru, M., & Sebastian, N. (2022). Comfort evaluation of ZnO coated fabrics by artificial neural network assisted with golden eagle optimizer model. Scientific Reports, 12(1), 1-16.

xiii. Amor, N., Noman, M. T., Ismail, A., Petru, M., & Sebastian, N. (2022). Use of an artificial neural network for tensile strength prediction of nano titanium dioxide coated cotton. Polymers, 14(5), 937.

xiv. Barbosa, J. A., Freitas, V. M., Vidotto, L. H., Schleder, G. R., de Oliveira, R. A., da Rocha, J. F., ... & Lima, R. S. (2022). Biocompatible Wearable Electrodes on Leaves toward the On-Site Monitoring of Water Loss from Plants. ACS Applied Materials & Interfaces.

xv. Marenco, L. F. L., de Oliveira, L. P., Vale, D. L., & Salles, M. O. (2021). Predicting Vodka Adulteration: A Combination of Electronic Tongue and Artificial Neural Networks. Journal of The Electrochemical Society, 168(11), 117513.

xvi. Zhang, J., Xin, P. L., Wang, X. Y., Chen, H. Y., & Li, D. W. (2022). Deep Learning-Based Spectral Extraction for Improving the Performance of Surface-Enhanced Raman Spectroscopy Analysis on Multiplexed Identification and Quantitation. The Journal of Physical Chemistry A, 126(14), 2278-2285.

xvii. Ferreira, L. F., Giordano, G. F., Gobbi, A. L., Piazzetta, M. H., Schleder, G. R., & Lima, R. S. (2022). Real-Time and In Situ Monitoring of the Synthesis of Silica Nanoparticles. ACS sensors, 7(4), 1045-1057.

xviii. Mandal, S., Paul, D., Saha, S., & Das, P. (2022). Multi-layer perceptron for detection of different class antibiotics from visual fluorescence response of a carbon nanoparticle-based multichannel array sensor. Sensors and Actuators B: Chemical, 360, 131660.