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Dense Neural Network For Optimal Prediction Of Bioactivity In Essential Oil-Producing Plants

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Abstract:

Now a days this deep learning technique is playing a vital role in different science sectors and also in biological fields.This technique is being implemented because it is good at deploying big data which are syllabified for processing non-linear and complicated relationships.The main aim of this research work is to predict the biological actions of the essential oil producing plants and also to classify them in subject to their chemical compositions by implementing Convolutional Neural Networks which is one of the deep learning technique. This study is based on the chemical content present in the Egyptian essential oil plants and their activities.As like the one more algorithm is also used on essential oil dataset called Multiclass Neural Network(MNN). The main concept of our study is to CNN algorithm.while testing using both the algorithms CNN and MNN is 98.13% and 81.88%.At the end this CNN model have been taken as the reliable model for analysing the bio activities of the Egyptian EC-containing plants.At last we would get 97% approximately as the prediction.

Keywords: Convolution Neural Network, Essential Oil, Multiclass Neural Network, deep learning,bioactivities.

Introduction

Artificial Intelligence is being implemented in day-to-day routine in order to reduce the difficulties for the humans. This includes Medical,Engineering and Biological domains like genomic and studies in promatic which are termed as complex and also non-linear.Deep learning is one off the main technique in Artificial Intelligence which having more number of new features from large datasets that are generated from genomics,Chemistryetc.,

Essential Oils (EOs) are biologically active chemical molecules derived from various sections of fragrant plants, including flowers, leaves, and barks. In complementary and alternative medicine, these natural compounds are extensively employed (CAM). Natural alternatives to inorganic chemistry continue to be a popular topic in modern research in biology.The reason behind this is usage in industries related to health like Medicine,pharmaceutics,edible things and liquids.As a result, modern research is focusing on finding alternative natural products, such as EOs,whenever human body feels an abnormal effects they can adopt because of higher potential.

These Essential Oil producing plant is categorised by their chemical structure and its concentration of Essential Oilsand that have the major influence in plants' biological functions.Essential oils are made by combining lower nuclear weighted natural material mixing to pure organic motility.

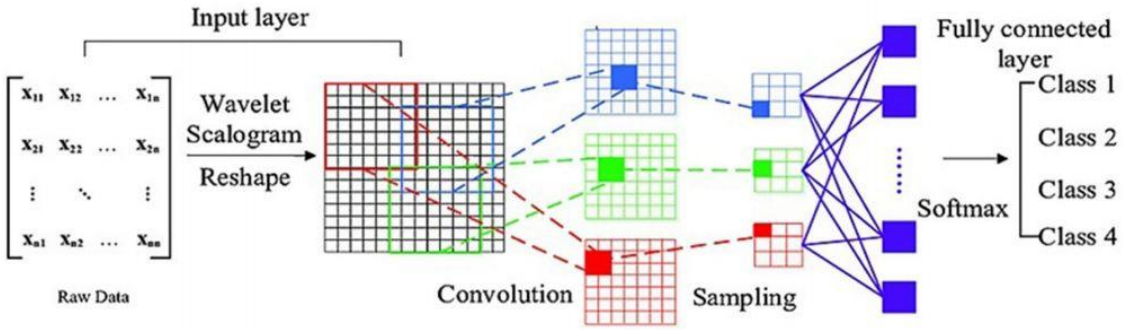

Fig 1: Common CNN Architecture

Now a days, to solve biological problems using Machine Learning algorithm some varieties of techniques are imposed partially Artificial Neural Network (ANN).ANN is an particular structure of numerical model with separate components for processing constructed between layers. These layers are made of secret neurons and these neurons lies between the intermediate layers they plays an important role in input and output processing in connection with neighbouring neurons in nearby layers.

Deep learning algorithms, on the other hand, are no longer limited to the image processing domain; they are already being regarded an appealing solution for various types of text classification issues, such as DNA sequence classification. Deep learning can be an effective learning method for dealing with the complicated composition of chemical compounds and their interrelationships with biological activity from this perspective.

As an experimental case study, this work aims to categorise and predict the biological activities of Egyptian essential oil-producing plants based on their EOs content. To test the efficiency of both machine and deep learning techniques, the classification is implemented using two algorithms: Multiclass Neural Network (MNN) and Convolution Neural Network (CNN). The efficient technique was used to create a biological activity prediction model for EOs-producing cases grown in Egypt.

The following are the research skills in this study: first, showing the outcomes of applying the two algorithms, MNN as a machine learning algorithm and CNN as a deep learning algorithm, using the Egyptian essential oils dataset. The results were then analysed and compared for the existing dataset as well as the new untested datasets. Finally, the methods used in this research are addressed.

Methodology:

The convolution layer, which applies a constitutional process on the input matrix, is the first of the subsequent successive layers. Each filter's convolution operation produces the output of each node in the convolution layer. The pooling layer is the next layer, and it compresses data and generalises features to reduce overfitting of the training data. The local max-pooling method is utilised in this experiment, which produces the maximum value from small divided sections in the input matrix.

$$O_s^d = \sum b_s^d + h_s^d + c_s^d$$

Here the O_s^d be the output vector of d^{th} layer and k^{th} kernel,b_s^d be the input vector,h_s^dbe the weight of convolution,c_s^d be the coefficient of bias.

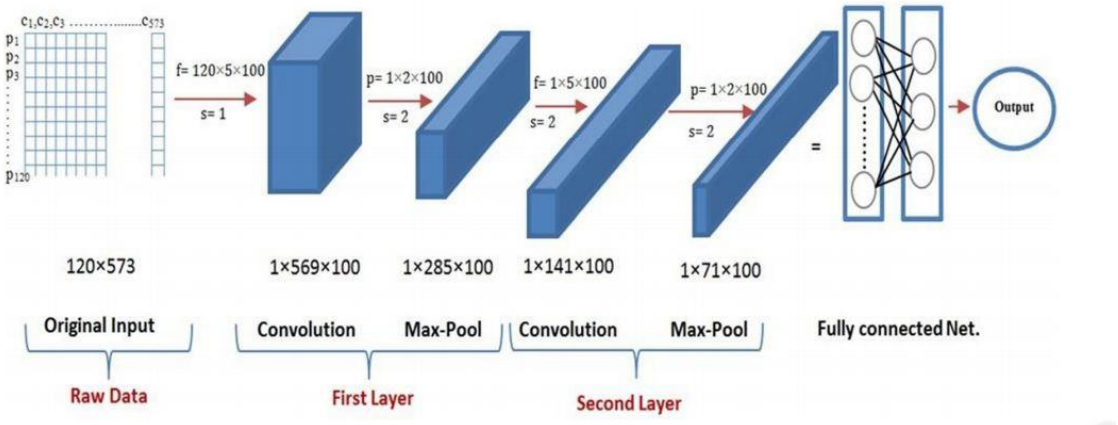

Fig 2 : The Proposed Building's Architecture CNN starts with a unique input matrix that reflects the essential oils data. Two layers of convolution and pooling make up the internal network structure. These layers' output is fed into a fully linked feed forward neural network.

Layers	Filter	Pace	O/P Size	O/P Dense
Input	-	-	120×573	68,760
Layer 1 of convolution	120×5×100	1	1×569×100	56,900
Layer 2 of convolution	1×5×100	2	1×141×100	14,100
1st Maxpooling Layer	1×2×100	1	1×285×100	28,500
2nd max pooling Layer	1×2×100	2	1×71×100	7100

Table 1 : CNN layers description hyper parameter values

This Table 1 explains the hyper parameter and output layer dimension.

$$p^d \times q^d = \left[\left[\frac{p^{d-1} - d^{d-1}}{s^d}\right] + 1\right] \times \left[\left[\frac{q^{d-1} - d^{d-1}}{s^d}\right] + 1\right]$$

The convolutional and pooling layers are then followed by a fully connected feed-forward neural layer with a "sigmoid" activation function. The sigmoid function was chosen for the suggested CNN implementation because its major job is to turn each score of the last node into a probability value between 0 and 1, regardless of the other scores. As a result, the input might be divided into several distinct classes.

Results and Discussions:

Tables 2 and 3 summarise the outcomes of the classification process for both the MNN and CNN algorithms. The training methods for the CNN and MNN algorithms exhibit overall accuracy of 100 percent and 99.2 percent, respectively, in correctly classifying essential oils activity. In the testing stage, CNN and MNN achieved overall accuracy of 98.13 percent and 81.88 percent, respectively.

Bio activity class Matrices	Possible Accuracy		Precision		Recall		F1 Score	
	MNN	CNN	MNN	CNN	MNN	CNN	MNN	CNN
Antiviral	0.72	0.99	0.9	0.98	0.5	0.99	0.64	0.99
Anticancer	0.9	0.94	0.96	0.93	0.86	0.94	0.9	0.94
Antimicrobial	0.73	0.97	0.7	0.97	0.79	0.97	0.74	0.97
Antifungal	0.84	0.99	0.86	0.99	0.812	0.98	0.83	0.99

Table 2: In the testing stage, the accuracy and relevance measures for MNN and CNN algorithms.

Bioactivity class Classifiers	True Possitive	True Negative	False Possitive	False Negative
Antiviral	98%	96.3%	3.7%	2%
Anticancer	97%	94.7%	5.3%	3%
Antimicrobial	94%	93.5%	6.5%	6%
Antifungal	100%	96.6%	3.4%	0%

Table 3: Confusion Matrix predicting model

The confusion matrix is the best method for validating categorization results. The MNN and CNN classification confusion matrix is shown in Table. True Positive, False Positive, True Negative, and False Negative are the four binary classifier outputs. Furthermore, multiple metrics such as accuracy, precision, recall, and F1 score are utilised to evaluate the classification efficiency based on the values of the confusion matrix. Table shows the four bioactivities metrics that have been calculated and documented.

Prediction Model for EO bioactivity using CNN-based prediction model:

The CNN algorithm shows great accuracy for the training and testing stages after the classification phase is completed. This is owing to its strengths in dealing with large amounts of data and focusing on the dataset's high-impact attributes. As a result, the CNN suggested method was used to create the biological activity prediction model. The overall accuracy for estimating the biological actions of previously unknown Egyptian essential oil components was around 97 %.

Conclusion:

Because of their efficacy as antiseptics, antimicrobials, antifungals, antioxidants, anticancer, antivirals, and anti-inflammatories, EOs are receiving a lot of interest from the health-related industries, such as medicine, pharmaceutics, and cosmetics. Traditional in-vitro investigations, on the other hand, face a significant barrier in determining the connection between the chemical components that make up the EO and its biological actions. As an experimental study case, two classification models are used to classify and predict the biological activities of 120 varieties of Egyptian essential oils.In order to examine the efficiency of both machine and deep learning techniques, this experiment was implemented using two types of supervised learning algorithms: Multiclass Neural Network and Convolutional Neural Network. In the testing stage, a comparison of the accuracy and relevance metrics for both the MNN and CNN algorithms revealed that the CNN outperformed the MNN, with an accuracy rate of 98.13 percent vs 81.88 percent for the MNN.

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