AI 4 Science Discovery Network+

Group: 16
Challenge: Task 3 - Detect defects in electron microscopy images
AI4SD ML Summer School Report
20-24th June 2022

Project Team: Xuerui Guo (University of Southampton), Zien Ma (Cardiff University), Jayanta Kumar Pal (University of Liverpool)

Report Date: 08/07/2022

AI4SD-SummerSchool-Series:Report-8

Group: 16
Challenge: Task 3 - Detect defects in electron microscopy images
AI4SD-SummerSchool-Series:Report-8
Report Date: 08/07/2022
DOI: 10.5258/SOTON/AI3SD0251
Published by University of Southampton

Network: Artificial Intelligence and Augmented Intelligence for Automated Investigations for Scientific Discovery
This Network+ is EPSRC Funded under Grant No: EP/S000356/1

Principal Investigator: *Professor Jeremy Frey*
Co-Investigator: *Professor Mahesan Niranjan*
Network+ Coordinator: *Dr Samantha Kanza*

Contents

1 Project Details

Group Number	16
Challenge Name	Task 3 - Detect defects in electron microscopy images
Project Dates	20-24th June 2022
Website	Link to the code implemented in Google Colab

2 Project Team

2.1 Project Student

Name and Title	Xuerui Guo (Remote sensing technician)
Employer name / University Department Name	University of Southampton / Geography and Env. Science
Work Email	Xuerui.Guo@soton.ac.uk
Website Link (Linkedin)	https://www.linkedin.com/in/xuerui-guo-222b181a2/

Name and Title	Zien Ma (Postgraduate student)
Employer name / University Department Name	Cardiff University / Computer Science
Work Email	maz17@cardiff.ac.uk
Website Link (Linkedin)	https://www.linkedin.com/in/zien-ma-585ba11b4/

Name and Title	Jayanta Kumar Pal (Postdoctoral Research Associate)
Employer name / University Department Name	University of Liverpool / Computer Science
Work Email	jkpal@liverpool.ac.uk
Website Link (Linkedin)	https://www.linkedin.com/in/jkpit08/

2.2 Project Supervisor

Name and Title	Mahesan Niranjan (staff)
Employer name / University Department Name	University of Southampton / ISIS Chair, Electronics and Computer Science
Work Email	mn@ecs.soton.ac.uk
Website Link (Linkedin)	https://www.linkedin.com/in/mahesan-niranjan-9226a713/

2.3 Challenge Description

Our task is to design a model automatically detect defection in several graphene Sheets.From 256*256 whole graphene sheet, 48*48 subset patches are generated, see figure1. 32 patches of defected cases and 2279 patches of non-defected cases with ground truth information are provided. The defected patches are labelled as 1 and the non-detected ones are labelled as 0.

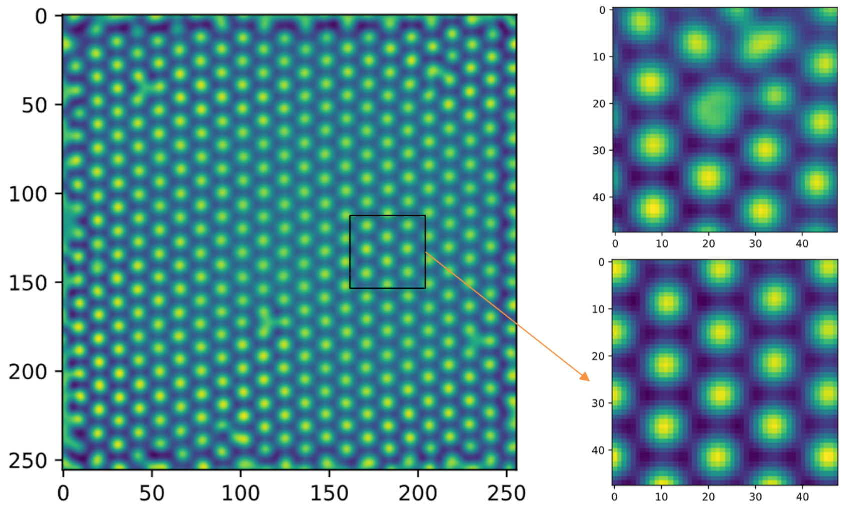

Figure 1: Visualize of 256*256 electron microscopy and its 48*48 subset patches, right side give two examples of defected (upper) and non-defected (lower) cases.

3 Theoretical background

Convolutional Neural Network (CNN) is a feed-forward neural network. In order to have a better understanding on its structure, we will first introduce its foundation: artificial neural network.

3.1 Artificial Neural Network [1]

Artificial Neural Network (ANN), also referred to as Neural Network (NN) or Connection Model, is an algorithmic mathematical model for distributed parallel information processing that mimics the behavioral characteristics of animal neural networks. This type of network relies on the complexity of the system to process information by adjusting the relationship between a large number of internal nodes connected to each other. Each node represents a specific output function, called the activation function. Each connection between two nodes represents a weighted value for the signal passing through that connection, called the weight. The output of the network varies depending on how the network is connected, the weight value and the activation function [1]. The idea of its construction was inspired by the functioning of the neural networks of living beings (human or other animals). Referring to the biological structure of neurons, McCulloch and Pitts [2] proposed an artificial neuron model, the M-P neuron model, in 1943, with the structure in the Figure 2.

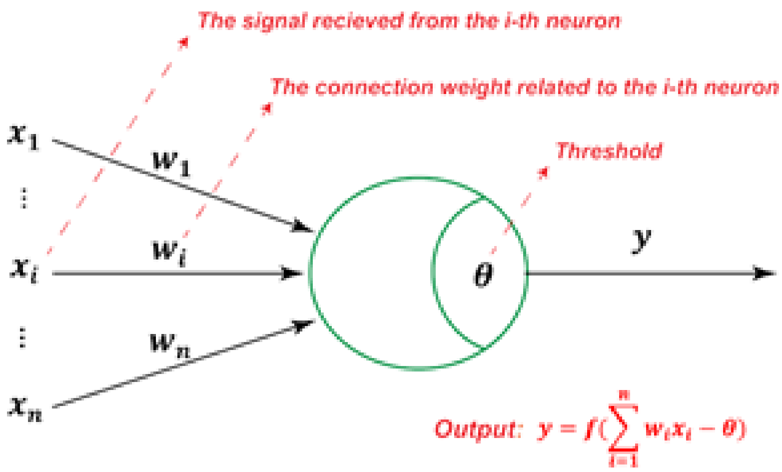

Figure 2: A mathematical neuron model. From [2]

On top of this mathematical model, more complex structures such as single-layer perceptrons are proposed, and the weights and threshold in the model are no longer fixed values, which gives it the ability to learn [3].

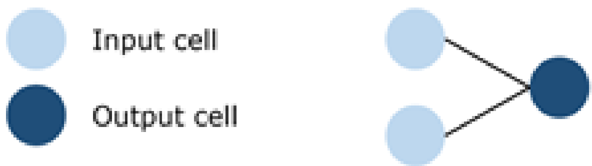

Figure 3: A single-layer perceptron

A hidden layer is introduced into the single layer perceptron, thus forming the well-known neural network structure.

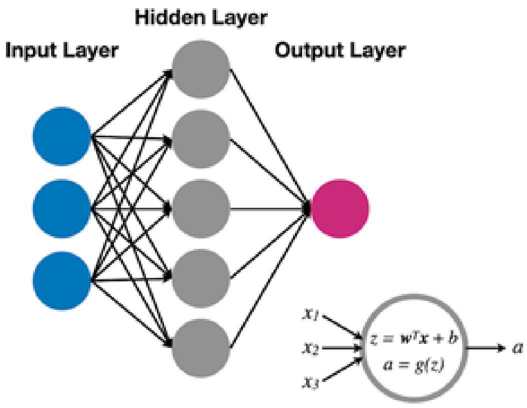

Figure 4: A artificial neural network, From [4]

3.2 Convolutional Neural Network [3]

The convolutional neural network [3] is a type of deep neural network with a convolutional structure. The basic idea of deep neural networks is to obtain better feature robustness by constructing multi-layer networks with the multi-layer representation of the target with a view to representing the abstract semantic information of the data through multi-layer high-level features. The convolutional structure can reduce the amount of memory occupied by the deep network, and its three key operations, one is the local perceptual field, the other is weight sharing, and the third is the pooling layer, effectively reducing the number of parameters of the network and alleviating the overfitting problem of the model.As you can see from this illustration in figure 5, a convolutional neural network consists of an input layer, a convolutional layer, a pooling layer, a fully connected layer, and an output layer.

3.2.1 The input layer

The input layer is the input to the whole neural network, which generally represents the pixel matrix of an image in a CNN that processes images. For example, in the figure 5, the length and width of the left matrix (32*32) represent the size of the image, while the depth of the matrix represents the color channel of the image. The depth of a black and white image is 1, while in RGB color mode, the depth of the image is 3.

3.2.2 The convolutional layer [5]

The convolutional layer is the most important part of a CNN. Unlike traditional fully connected layers, each node in the convolutional layer has only a small piece of input from the previous layer of the neural network, either 3*3 or 5*5. The convolutional layer tries to analyze each piece of the neural network in greater depth to obtain more abstract features. The convolutional layer will make the node matrix deeper after a set of process.

3.2.3 The pooling layer [5]

The pooling layer can reduce the size of the matrix. The pooling can be considered as transforming a higher resolution image into a lower resolution image. By pooling, the number of nodes in the final fully connected layer can be further reduced, thus achieving the goal of reducing the parameters in the whole neural network.

3.2.4 The fully-connected layer [5]

There are usually one or two fully connected layers at the end of the CNN. The information in the image is considered to be abstracted into features with higher information content. Convolutional and pooling layers can be considered as the process of automatic image feature extraction. And the classification or regression task is carried out by the fully connected layer.

3.2.5 The output layer

The last output layer is an activation function depending on the task is regression or classification. In this case (the figure 5), the Softmax layer is mainly used for classification problems. After the Softmax layer, the probability distribution of belonging to different kinds in the current sample can be obtained.

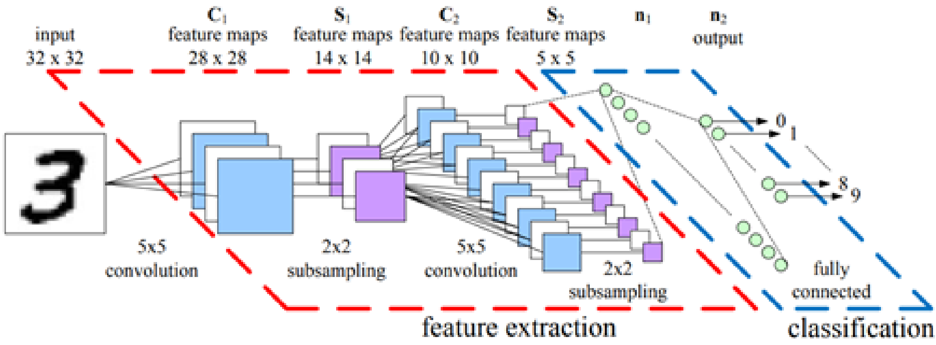

Figure 5: A example of convolutional neural network

4 Methodology

In our case, we performed defect detection using 2D CNN, because CNN is proven to outperform in classification and the defect and non-defect detection is a typical binary decision classification. The model structure design as shown in Figure 6). We used in total 4 convolution layers and 3 max pooling layers, the kernal size is 3*3 and Max polling size is 2*2. We set batch size to 32 and the evaluation metrics is accuracy ,besides, 'Binary cross-entropy' is used as the loss function and 'adam' is used as the optimizer.

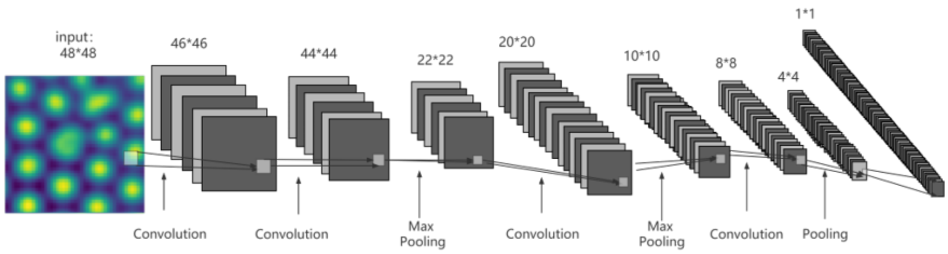

Figure 6: Customised 2D-CNN model structure for graphene detection

5 Result and discussion

In our investigation we used 100 epochs for training and validation. From Figure 8), it is evident that the loss of our 2D CNN model is sharply decreasing for both the cases of training and test/validation set.Figure 7)shows the improvement of accuracy with the forward direction of epochs. It is observed from this figure that for both the training and testing/validation set the accuracy is sharply increasing with the increasing number of epochs. Two suggestions for the future researches: First is to increase the dataset.Through nice results have achieved by 2D-CNN model, the saturated accuracy line indicate the overfitting with limit amount of the training data. Second is to add more information of the images. In our case, only a binary of 0 or 1 are given per subset patch, if we could involve in more colour channels (RGB), it could provide more detailed information and a CNN with more dimensional could be used.

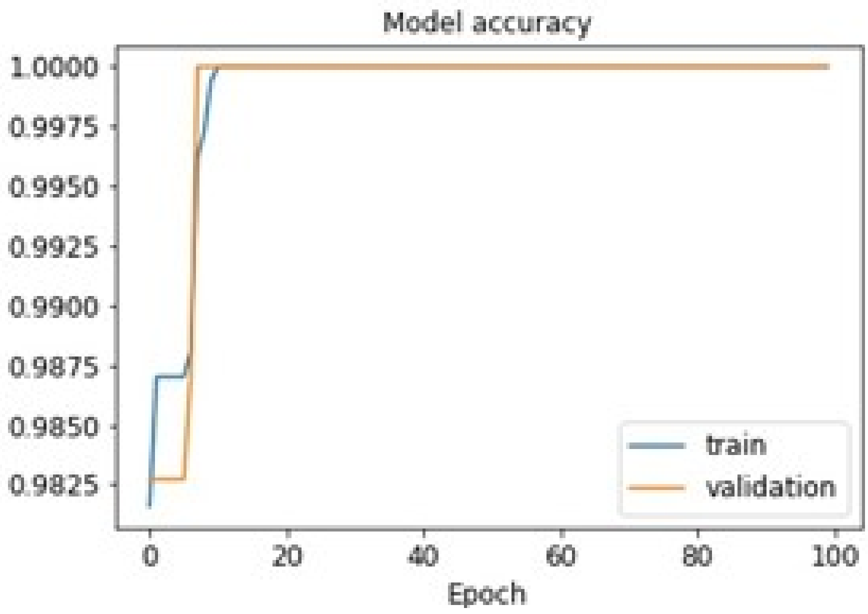

Figure 7: Increase of accuracy with epochs

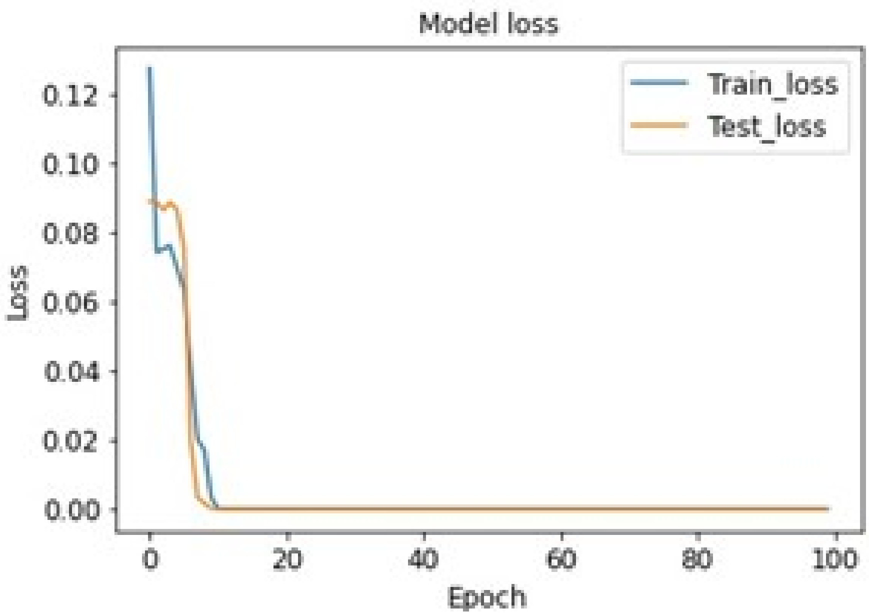

Figure 8: Decrease of loss with epochs

References

[1] Ng A. CS 229 Lecture notes at Stanford University; 2022. Available from: https://see.stanford.edu/course/cs229.

[2] Mcculloch WS, Pitts W. A LOGICAL CALCULUS OF THE IDEAS IMMANENT IN NERVOUS ACTIVITY; 1943.

[3] Ma Z. Literature Review for 9-month Review in COMSC School of Cardiff University; 2022.

[4] Christian. A shallow neural network for simple nonlinear classification; 2022. Available from: https://scipython.com/blog/a-shallow-neural-network-for-simple-nonlinear-classification/.

[5] Processing S, Systems Proceedings of the 8th International Conference on Communications SP, Systems. Lecture Notes in Electrical Engineering; 2020.

List of Figures