

Neural networks homework assignment with hands-on activities

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The following problems will help you understand how to perform classification tasks with neural networks. You will learn how to process training data as well design networks with activation functions and objective functions to perform a classification task. You will learn how to interpret the output of the network and quantify network performance using metrics such as accuracy. Before starting with the assignment make sure you go over the accompanying lecture and hands-on tutorial. For the assignments below, you will work with the *Neural Network Classification to predict crystal structures* notebook in the following tool: <https://nanohub.org/tools/mseml>

Problem 1. The learning module example showed a neural network to classify elements into FCC, BCC or HCP crystal structures. Let's say we now wish to classify elements into FCC, BCC, HCP or Simple Cubic crystal structures. To train this network we need to map these classes to one-hot vectors. Write down one-hot encodings for each of these categories, and write down the one-hot encoding for copper (Review slide 13 for one-hot encoding | Copper has an FCC crystal structure)

Problem 2. What activation function is used in the last layer of the network in the learning module? Write down the equation of this activation function, and the maximum and minimum values this function can take. Continuing with our previous example, let's say the output of our network for copper is [0.2, 0.3, 0.4, 0.1]. What is the predicted crystal structure for copper?

Problem 3. In this network we use accuracy as a metric to define the success of our network. Write down the equation for accuracy. What is the accuracy of the network in the learning module on the training and testing datasets?