Determination of Crystal Structure using Artificial Intelligence

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Objective: Use convolutional neural networks to predict the crystal system, extinction group and space group of completely unknown inorganic materials using its powder XRD pattern.

Deep Learning

Artificial Intelligence (AI) involved the development of self-learning algorithms to gain knowledge from data in order to make predictions. One of the algorithms that it uses are Neural Networks (1).

Neural Networks receive input data and transform it through a succession of hidden layers. Each layer has a number of neurons that collect information from the previous layer. This information is converted into a specific value by using an activation function to be transferred to neurons in the next layer (2). The activation function is applied to a linear combination between the information of the previous layer and independent variables defined by the network (weights and biases).

For a regular Neural Networks, the most common layer type is the fully-connected in which neurons between two adjacent layers are fully pair wise connected. It is called fully feed forward neural network (2).

The goal in Supervised Learning is to learn a model from labeled training data (a set of samples where the desired output labels are already known) that allows us to make predictions.

Deep Learning is a set of techniques for learning in neural networks implemented with more than one hidden layer (3).

An application of neural networks is the classification, whose central idea is to determine the class (label) to which the input data that belongs to network.

When the network predefines the independent variables it is called a Convolutional Neural Network (CNN).
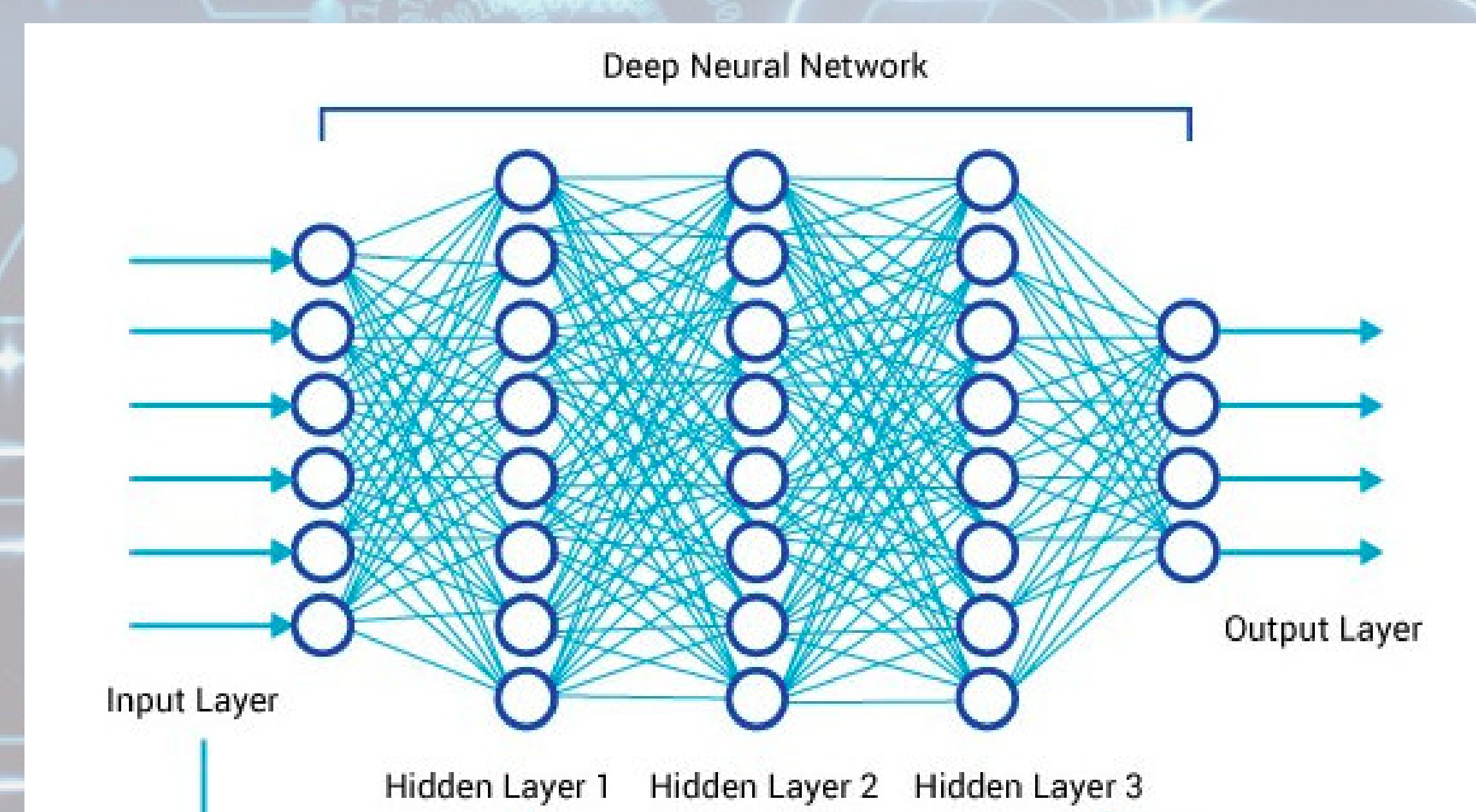

Figure 1. Deep Neural Network. .

Convolutional Neural Network

A Convolutional Neural Network is made up of two parts. The first is formed with a series of convolution and pooling layers; and the second corresponds to a fully feed forward neural network.

The convolution layer detects features through a series of filters and the pooling layer reduces the spatial resolution, which allows working with deeper networks.
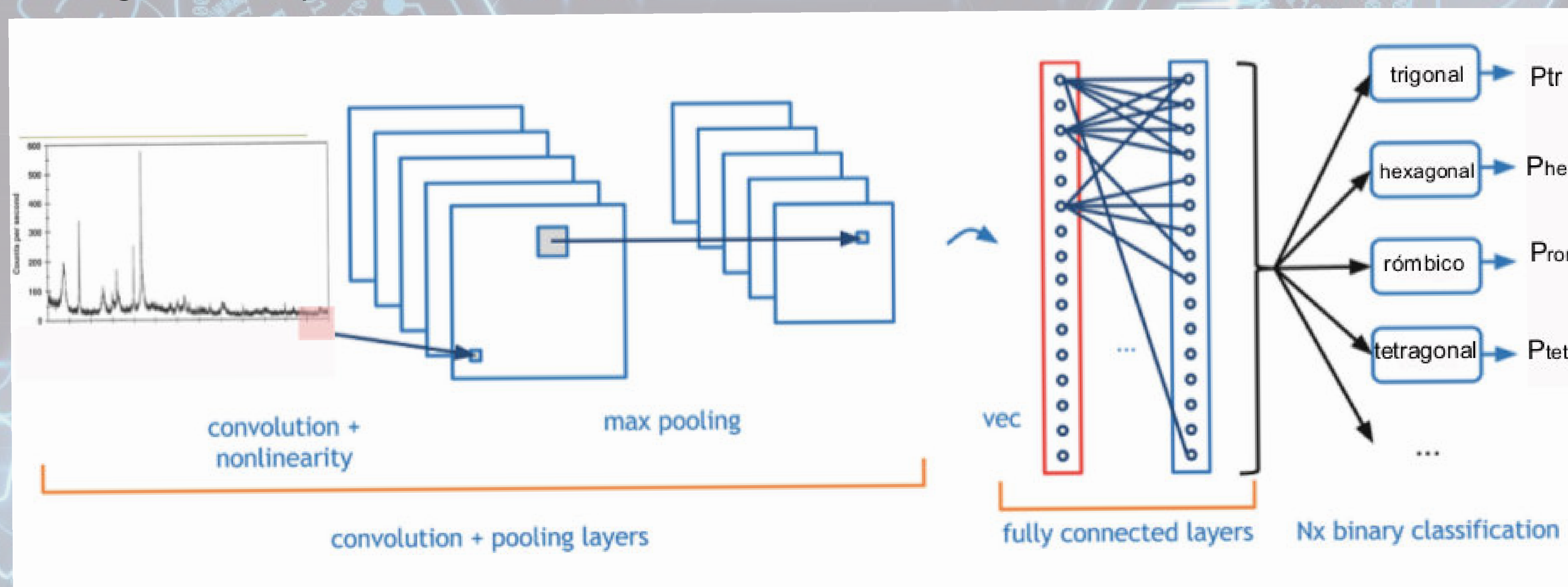

Figure 2. Convolutional Neural Network**.**

Development

More than 100,000 powder XRD patterns of inorganic compounds will be modeled, which will be used as input to a CNN. The network will be designed to characterize inorganic compounds whose crystal structure is unknown. The classes that are going to use in the networks are crystal system, extinction group and space group. Finally powder XRD patterns of unknown inorganic compound will be measured and with CNN trained its crystal system, extinction group and space group will be predict. For each classification a), b) and c) a different network will be made (Fig. 3).
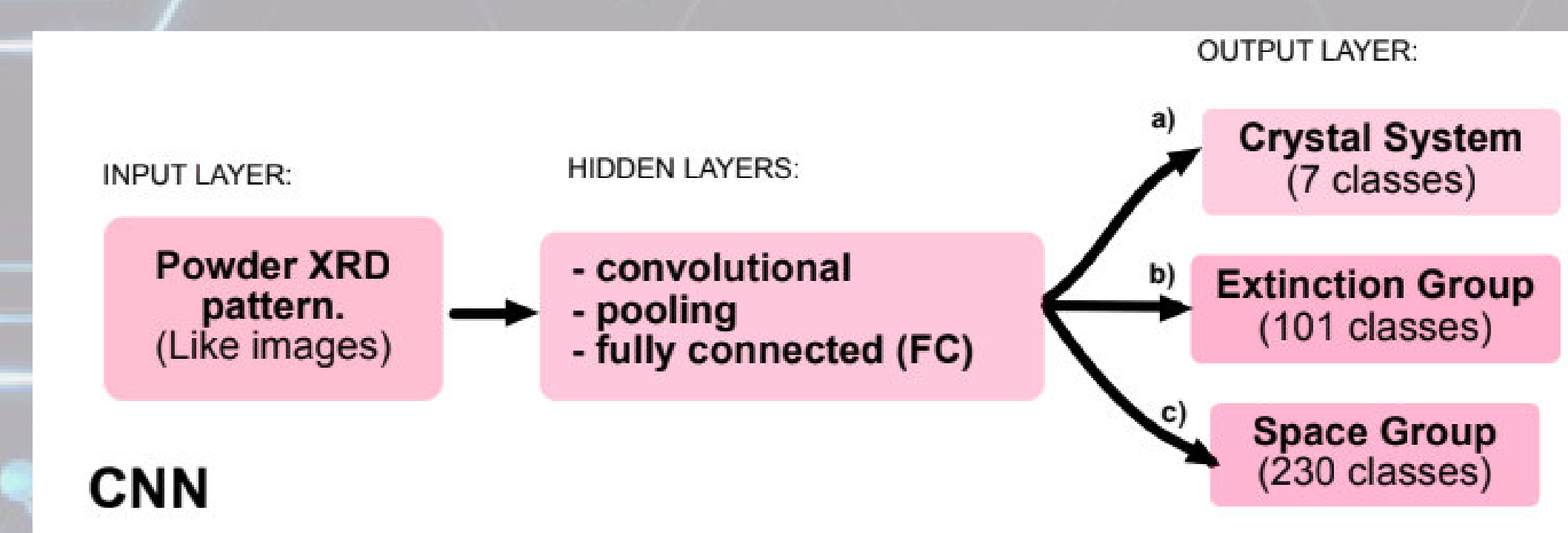

Figure 3. CNN diagram.

References

(1) Raschka, Sebastian. **Python Machine Learning**. Open source, Birmingham-Mumbai, 2015.

(2) W. B. Park, J. Chung, J. Jung, K. Sohn, S. P. Singh, M. Pyo, N. Shin, K-S. *Sohn. Int. U. Crys. J., 4,* **2017,** 486-494.

(3) Ng, Andrew. **Specialization in Deep Learning** (Coursera).