Atomic coordinate prediction of carbon nanotubes with NNs

1 Description

ML algorithms are increasingly applied in Physics [1, 2, 3]. The objective of this project is to predict the atomic coordinate prediction of carbon nanotubes from a reduced number of nanotubes attributes. The dataset was generated using an algorithm that simulates a wide range of properties of materials proprieties [1].

The dataset is available from[1]. The original publication [1] provides details of the dataset.

2 Objectives

The goal of the project is the application of Neural Networks for: I) Predicting the three coordinates of the nanotubes. II) Implement a multi-layer perceptron for this problem and compare it to one or more classifiers not based on NNs.

The student should: 1) Implement the solution of the prediction problem (simultaneous regression of the three coordinates). 2) Evaluate and discuss the results of the regressor:

As in other projects, a report should describe the characteristics of the design, implementation, and results. A Jupyter notebook should include calls to the implemented function that illustrate the way it works. The report should explain the feature engineering approach, describe the validation process, and show tables or figures with the accuracy of the classifiers.

3 Suggestions

- The use of tensorflow or keras is recommended.
- Be aware that this is a regression problem.
- Implementations can use any other Python library.

References

[1] Mehmet Acı and Mutlu Avcı. Artificial neural network approach for atomic coordinate prediction of carbon nanotubes. *Applied Physics A*, 122(7):631, 2016.

[2] P. Pakzad and V. Anantharam. Belief propagation and statistical physics. In *Electronic Proceedings of 2002 Conference on Information Sciences and Systems*, Princeton University, 2002. Paper No.225, CD-ROM, 3 pages.

[3] Maria Schuld, Ilya Sinayskiy, and Francesco Petruccione. An introduction to quantum machine learning. *Contemporary Physics*, 56(2):172–185, 2015.

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[1]http://archive.ics.uci.edu/ml/datasets/Carbon+Nanotubes