Can an Artificial Intelligence do Science ?

Raphaël-David Lasseri*
ESNT, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France

David Regnier† and Jean-Paul Ebran‡
CEA, DAM, DIF, 91297 Arpajon, France

Guillaume Hupin§
Institut de Physique Nucléaire, Université Paris-Sud, IN2P3-CNRS, Université Paris-Saclay, F-91406 Orsay Cedex, France

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I. SCIENTIFIC ISSUE

Atomic nuclei provide a beautiful example of a complex quantum many body system that exhibits emergent orders and cooperative behaviors such as superfluidity or molecular clustering. The consistent theoretical description of these features is still a challenge after several decades of research. The difficulties inherent to the non-perturbative nature of quantum chromodynamics at the typical scales involved in nuclear physics on the one hand, and to the treatment of the many-body problem on the other hand, hinder the formulation of a high-fidelity theoretical picture of nuclear properties. Typically, the description of nuclei with ab initio techniques is still limited to a few percent of the nuclides chart. Opting for other relevant degrees of freedom is a possible strategy. Along this line, empirical nuclear EDFs (Energy Density Functionals) seem to indicate a powerful language to encode the diversity of nuclear phenomenology in an efficient way. Unfortunately, they still show several flaws in their state of the art formulation and applications.

In a time of exponential development of the field of machine learning, it is worth seeking how the rich set of methods of this discipline could be leveraged to overcome the current challenges of nuclear physics. As the community is establishing the first bridges between these two domains of research, we may boldly ask ourselves: Is a machine able to understand (almost) on its own the physics of the nuclei ? More generally, how does a machine see and represent the laws of our universe ? These questions are shared among a variety of scientific communities as more and more artificial intelligence applications in physics show promising results. However these approaches are frequently considered as "black-boxes" which is both an important technical and philosophical issue.

In this context, the aim of this workshop is to bring together scientists from different fields (chemistry, statistical physics, nuclear and particle physics, biology, cosmology, etc) to share their experience and successful applications of machine learning. It will be the occasion to discuss the benefits and perspectives of artificial intelligence for nuclear physics as well as the common pitfall and limits of its application in physics and society. This workshop is organized by the Espace of Structure and Nuclear reaction Theory (ESNT), and is supported by the CEA, DAM and CEA, DRF.

References

Machine Learning:

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*Electronic address: raphael.lasseri@cea.fr
†Electronic address: david.regnier@cea.fr
‡Electronic address: jean-paul.ebran@cea.fr
§Electronic address: hupin@ipno.in2p3.fr

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Artificial intelligence and Physics:

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II. GOALS

The main goals of this workshop are to :

- Establish a global overview of state-of-the art Machine Learning Techniques, which may lead to progress in our fields of research;
- Initiate a large scale effort towards application of Neural Networks to nuclear Many Body Problem;
- Establish a "task-force" to promote these approaches and study their epistemological implications;
- Give epistemological and societal insights of the massive development of Artificial Intelligence;

III. TENTATIVE PROGRAM

Structure

The meeting takes place over the week. The first day is devoted to introductory/pedagogical presentations that have the aim of informing/educating the local research community. The following days will be more focused on the specificities of IA.

Introductory Lectures

1. Stephane Mallat *General Overview of AI Application to Scientific Fields*
2. Yann Lecun *Deep-Neural Network: Foundations and Perspectives*
3. Yoshua Bengio *Deep Learning and Generative Techniques*

Scientific talks

- Jean-Paul Ebran *The Nuclear Many-Body Problem*
- David Rousseau *Generative Networks for High Energy Physics*
- Andrew Senior *Protein structure prediction using potentials from deep learning*
- Justin S. Smith *DFT and neural network*
- Giuseppe Carleo *Solving the Quantum Many-Body Problem with Artificial Neural Networks*
- Simona Cocco *Machine learning protein sequences*
- Lenka Zdeborová *Bridges betweeen statistical physics and machine learning*
- Alberto Rosso *Alberto Rosso*

- Jean-Marc Martinez *An extensible neural network potential with DFT accuracy at force field computational cost*
- J.B Maillet *Machine learning potentials in material science*
- P. Mutti *Artificial Intelligence Applied to Photon and Neutron Science*
- B. Després *Machine Learning in numerical schemes for compressible flows dynamics*
- Alessandro Pastore *Gaussian Processes and Machine Learning techniques applied to nuclear structure*
- Andrea Idini *PAC Learnable Nuclear Physics*
- Thomas Papenbrock *Extrapolation methods based on artificial neural networks for nuclear observables*
- Guillaume Hupin *Guillaume Hupin*
- Richard J. Furnstahl *Bayesian methods and machine learning*
- R. Lasseri D. Regnier *Taming nuclear complexity with a committee of multilayer neural networks*
- Amy Lovell *Machine learning in nuclear data evaluation*
- Cédric Villani *Cédric Villani*
- Vincent Bontems *Ethics of artificial intelligence*
- Bernard Stiegler *Artificial intelligence: progress or social regression*