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UNRAVELLING NEURAL NETWORKS WITH STRUCTURE-PRESERVING COMPUTING

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ABSTRACT

The understanding of processes and phenomena in science and engineering is radically transformed by machine learning. Many scientists and engineers embrace machine learning as an important tool. At the same time, obstacles and challenges are becoming apparent: most machine learning approaches require large amounts of data, but in many applications data is scarce. Furthermore, the performance and reliability of artificial neural networks − the dominant type of 'learned machines' − is usually difficult to interpret. To overcome this issue, the use of prior knowledge is key.

The *ultimate goal* of this mini-symposium is: to reveal how neural networks can be made more effective and efficient, and better understood, by incorporating mathematical and physical knowledge into their design. The *direct goal* of the mini-symposium is to contribute to the development of theory for mimetic neural networks for data-efficient and well-understood machine learning in computational science and engineering.

To achieve the above, it is necessary to have contributions from multiple disciplines. For this reason, the mini-symposium will have expert speakers from mathematics, computer science, machine learning, physics and astronomy.

From a mathematical point of view, there are many open questions. Overarching is the question: How can we optimally embed prior knowledge into neural networks? More specific questions are: How can we create interpretable machine-learning models? How can we further optimize training algorithms for neural networks? What are the nonlinear stability conditions and other requirements of neural networks?

Answers to these questions are very important for among others fluid mechanics and astro-mechanics, with essential opportunities for cross-pollination and mutual benefits for both. Work by astronomers on the N-body problem [1] demonstrates that neural networks can be used to make N-body computations, with N»1, much more efficient. In fluid mechanics, machine learning methods for the analysis, modelling, and control of turbulent flows are currently developed to answer both fundamental and applied questions. The intrinsic chaotic behaviour of multi-body systems in astro-mechanics resembles the non-trivial statistical properties of turbulence in fluid mechanics.

The mathematically inclined contributions to the mini-symposium will concentrate on fundamental properties of neural networks that potentially have a big influence on future methodologies for constructing neural networks to be used in computational science and engineering. The fluid mechanics and astro-mechanics contributions concentrate on specific challenges which serve as test cases for potentially more general strategies.

REFERENCES

[1] T. Boekholt and S. Portegies Zwart, “On the reliability of N-body simulations”, *Computational Astrophysics and Cosmology*, Vol. **361**, pp. 979-980 (2018).