

UNRAVELLING NEURAL NETWORKS THROUGH STRUCTURE-PRESERVING COMPUTING

TRACK NUMBER 1700

BARRY KOREN^{*}, BENJAMIN SANDERSE[†] AND WIL SCHILDERS^{*}

^{*} Eindhoven University of Technology
P.O. Box 513, 5600 MB Eindhoven, The Netherlands
b.koren@tue.nl, w.h.a.schilders@tue.nl

[†] Centrum Wiskunde & Informatica
P.O. Box 94079, 1090 GB Amsterdam, The Netherlands
b.sanderse@cwi.nl

Key words: Machine Learning, Neural Networks, Structure-Preserving Computing.

ABSTRACT

The development of simplified computational models of complex phenomena in science and engineering is an ongoing challenge. The purpose of such simplified models is typically to reduce computational cost at a minimal loss of accuracy. At the same time, more importantly, these models can provide fundamental understanding of underlying phenomena.

Last years, the following two concepts have gained significant importance in computational science and engineering: (i) *machine learning* (in particular neural networks) [5,8] and (ii) *structure-preserving (mimetic) computing* [3,7,9]. While neural networks are very strong as high-dimensional ‘universal function approximators’, they require large datasets for training and tend to perform poorly outside the range of training data. On the other hand, structure-preserving methods are strong in providing accurate solutions to complex mathematical models from science and engineering, but are typically computationally expensive (this can be reduced by using Model-Order Reduction).

The goal of this one-session mini-symposium will be: to better understand neural networks, to enable the design of highly efficient, tailor-made neural networks built on top of and interwoven with fundamental properties of the underlying science and engineering problems. The mini-symposium will address:

- Mathematical analysis and understanding of neural networks, e.g. modelling of neural networks in terms of differential equation solvers [1,4,6] or as Gaussian processes [2]. Dynamic neural networks will also be considered, and their relations to state-space representations [10].
- Design of novel neural networks with embedded invariance / enforced constraints, e.g. by adapting input features, neurons (activation function), network architecture, or cost function.
- Testing for some problems from science and engineering..

REFERENCES

- [1] R.T.Q. Chen, Y. Rubanova, J. Bettencourt and D. Duvenaud, “Neural ordinary differential equations”, *Proceedings 32nd Conference on Neural Information Processing Systems (NeurIPS 2018)*, Montréal, pp. 1-13, 2018.
- [2] A. Choromanska, M. Henaff, M. Mathieu, G. Ben Arous and Y. LeCun, “The loss surfaces of multilayer networks”, *Proceedings 18th International Conference on Artificial Intelligence and Statistics (AISTATS)*, San Diego, pp. 192-204, 2015.
- [3] S.H. Christiansen, H.Z. Munthe-Kaas and B. Owren, “Topics in structure-preserving discretization”, *Acta Numerica*, Vol. **20**, pp. 1-119, 2011.
- [4] W. E, “A proposal on machine learning via dynamical systems”, *Communications in Mathematics and Statistics*, Vol. **5**, pp. 1-11, 2017.
- [5] I. Goodfellow, Y. Bengio and A. Courville, *Deep Learning*, MIT Press, 2015.
- [6] E. Haber and L. Ruthotto, “Stable architectures for deep neural networks”, *Inverse Problems*, Vol. **34**, 2017.
- [7] B. Koren, R. Abgrall, P. Bochev, J. Frank and B. Perot (eds.), *Physics-Compatible Numerical Methods*, special issue *Journal of Computational Physics*, Vol. **257**, Part **B**, 2014.
- [8] Y. LeCun, Y. Bengio and G. Hinton, “Deep Learning”, *Nature*, Vol. **521**, pp. 436-444, 2015.
- [9] D. Pavlov, P. Mullen, Y. Tong, E. Kanso, J.E. Marsden and M. Desbrun, “Structure-preserving discretization of incompressible fluids”, *Physica D: Nonlinear Phenomena*, Vol. **240**, pp. 443-458, 2011.
- [10] W.H.A. Schilders, “Predicting the topology of dynamic neural networks for the simulation of electronic circuits”, *Neurocomputing*, Vol. **73**, pp. 127-132, 2009.