OTTO VON GUERICKE
UNIVERSITÄT
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VST

FAKULTÄT FÜR VERFAHRENS-
UND SYSTEMTECHNIK

Bachelor's or Master's thesis No.: LSS-M?
Task for the Bachelor's or Master's thesis of: ?

Neural networks for simulation of chemical reaction rates

Overall topic:
Artificial neural networks (ANN) have become incredibly popular in the last years, most often under the name of Deep Machine Learning. Our group had already the occasion to work with ANN several years ago (Fig.1, from Kuhn, R., Bordás, R., Wunderlich, B., Michaelis, B. and Thévenin, D.: Colour class identification of tracers using artificial neural networks. In: *10th International Conference on Engineering Applications of Neural Networks*, Thessaloniki, Greece, 13/2/1-8, 2007; So wie Emami, M.D. and Eshghinejadfard, A., Laminar flamelet modeling of a turbulent CH4/H2/N2 jet diffusion flame using artificial neural networks, *Applied Mathematical Modelling*, 36 (2012) 2082-2093), but the underlying procedures have undergone much progress recently. This is why it is interesting to check again the efficiency of current ANN for solving a problem of practical interest. The present project will assess the cost and accuracy of ANN for predicting chemical reaction rates in complex kinetic processes. The project will rely on the ANN implementation in Matlab, since recent studies have shown that it is very efficient. Reference data for training as well as for later testing will be provided by the exact solution obtained with the open-source software CANTERA.

Tasks in detail (will be adapted in the final version depending on Bachelor or Master level):
- Carry out synthetic literature study in the field of ANN for chemical reaction rates.
- Implement a working procedure for a simple configuration, like hydrogen oxidation.
- Check accuracy and numerical cost, as a function of number of layers and neurons, of size of training set.
- Prepare the way for more complex systems.
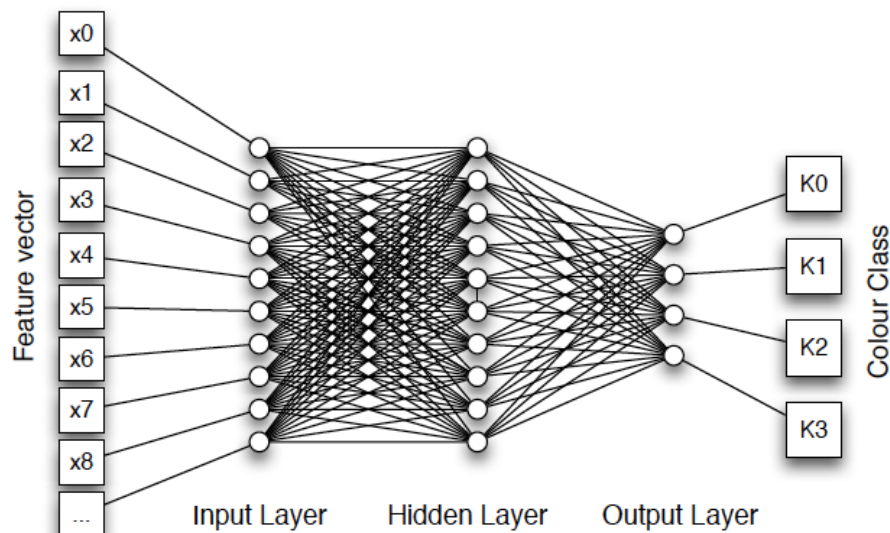
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Beginning: as soon as possible