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On the Prospects of Using Machine Learning for the Numerical Simulation of PDEs: Training Neural Networks to Assemble Approximate Inverses

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Machine Learning (ML) is a class of methods that can solve a multitude of problems by storing knowledge to and inferring it from a knowledge base that had previously been created via a training process. Due to its success the hardware industry and chip vendors adapt their roadmaps to satisfy an ever larger demand to computing hardware that is tailored for ML. The idea of this work is to exploit ML (and the modern and future compute hardware) for the simulation of PDEs by accelerating the linear solver: It is based on the observations, that (1) besides pattern recognition ML can also be used for *function regression* and (2) that preconditioners in linear solvers can be underdetermined and yet yield a good preconditioner: Sparse Approximate Inverses (SPAI) are a good representative of such a preconditioner. The application of an approximate inverse can be broken down to sparse matrix vector multiply (SpMV) and with sophisticated storage formats SpMV kernels map decently to for example GPUs. In contrast to that usual implementations of SPAI algorithms to *assemble* the approximate Inverse are (in spite of their good parallelisation properties) quite expensive. Hence the idea is to compute a rough draft of an explicitly stored preconditioner in a different way and therefore provide an alternative to SPAI: Use the system matrix as input to a trained neural network and render the result into another (sparse) matrix that is used as an approximation to its inverse. We use a Richardson iteration applying the approximate inverses generated by fully connected feed-forward multilayer perceptrons as preconditioners [1]. We provide insight into such a system based on different numerical experiments on the basis of the Poisson equation and concentrate on providing evidence that the resulting inverses can numerically compete with other preconditioners.

REFERENCES

[1] Hannes Ruelmann, Markus Geveler, and Stefan Turek. On the prospects of using Machine Learning for the numerical simulation of PDEs: Training Neural Networks to assemble Approximate Inverses. *ECCOMAS newsletter*, issue 2018, 2018. accepted.