Neural-Guided Equation Discovery: Episode 2

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Based on some desirable properties of equation discovery systems, we show why deep learning approaches are becoming increasingly attractive for equation discovery. We demonstrate the advantages and disadvantages of using neural-guided equation discovery by giving an overview of recent papers and the results of extensive experiments using our modular equation discovery system MGMT (**M**ulti-Task **G**rammar-Guided **M**onte-Carlo **T**ree Search for Equation Discovery) [1].

The system uses neural-guided Monte-Carlo Tree Search (MCTS) and supports both supervised and reinforcement learning, with a search space defined by a context-free grammar. The guiding network obtains for each state in the search tree the current equation and the data set for which the symbolic description is sought. The guidance is a distribution regarding which grammar rule to apply next. Within this scheme, we conduct experiments whose results can be summarized as:

(i) A search guided by neural networks provides results of the same quality with fewer visited states compared to a search without neural networks. (ii) Supervised training gives better results than MCTS-based training. (iii) Integrating tabular data set embeddings can improve the search, but simple architectures perform surprisingly well compared to more complex architectures. (iv) A grammar is an effective way to reduce the search space also in neural-guided equation discovery by using domain knowledge: Models have no difficulty using the rules from the grammar instead of tokens as output space.

At the end, we want to discuss three perspectives on the problem of equation discovery. The first perspective (i) is to understand it as a combinatorial problem, finding the right permutation of tokens for a data set as efficiently as possible with respect to the given resources (time, space, energy, ...). The second perspective (ii) is to consider equation discovery as a challenging example domain for deep learning. In deep learning, training and test sets are supposed to follow the same distribution in most domains. In contrast, equation discovery at the frontier of science is used for problems where previous experience may not be sufficient. A third perspective (iii) on equation discovery is that of a problem, where new knowledge is generated by using previously gained knowledge and the question if concepts, such as symmetries, integration, or energy conservation can be automatically derived and so far unknown concepts be discovered.

References

[1] Jannis Brugger et al. "Neural-Guided Equation Discovery". en. In: *(under review) Computational Approaches to Scientific Discovery* (2024).

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