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Machine Learning Methods for Cayley Graphs Path Finding and Embeddings

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We present the application of machine learning and reinforcement learning methods to the analysis of Cayley graphs, specifically focusing on path finding and graph embeddings. This approach is inspired by DeepMind's AlphaGo system. It is already able to overcome GAP (classical computer algebra system): we are finding paths on groups of orders 10ˆ40-10ˆ70, while GAP encounters computational limits for such large groups. The method is general and can be applied to any (finite) permutation or matrix group. Lengths of paths produced by our general approach are shorter than obtained by algorithmic and other solvers which can handle only specific groups like Rubik's Cube group. More generally we will argue that Cayley graphs provide an excellent framework for the mathematical understanding of the key concepts of modern machine learning and reinforcement learning in particular. If time permits we will describe potential applications of that technique to biological questions like construction of embeddings for proteins and drugs like small molecules.

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