Learning-based Strategies in Deterministic Global Optimisation of MINLP Models in Chemical Engineering

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This PhD project will focus on advancing deterministic global optimisation methods for mixed-integer nonlinear programming (MINLP) models in chemical engineering by integrating machine learning and reinforcement learning techniques. Deterministic global optimisation provides rigorous guarantees for handling the nonconvexities and combinatorial complexity inherent in MINLP formulations of process design, synthesis, and scheduling problems, but it often suffers from prohibitive computational cost. The project will explore how data-driven surrogates and learning-based strategies can accelerate key algorithmic components, such as bound tightening, branching decisions, cut generation, and the combination of effective relaxation techniques. In particular, reinforcement learning will be investigated to guide search strategies adaptively, improving efficiency in exploring the solution space while maintaining global optimality guarantees. By combining the reliability of deterministic optimisation with the adaptability of modern learning methods, this research aims to deliver scalable and agile optimisation tools and software that unlock new possibilities for computer-aided molecular and process design, enterprise-wide process optimisation, and sustainable process systems engineering.