PhD Research Proposal

Solving Mixed-Integer Problems by combining Reinforcement Learning and Artificial Evolution

Background : Master 2 in Computer Science, or Bioinformatics

Skills : Algorithmics, Python or Java programming, English reading & spoken

Laboratory : Laboratoire I3S, SPARKS team, UMR 7271 UniCA CNRS, 06900 Sophia Antipolis, France

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Scientific context. Mixed-integer optimization (MIO), which combines continuous and discrete variables, is a key area in operations research and artificial intelligence. It is used in complex problems where the variables to be optimized are not only continuous, such as weights or proportions, but also discrete, such as binary choices or integer assignments.

This type of optimisation is fundamental to a wide range of applications, such as planning and scheduling (production management, logistics), design of complex systems (engineering, communication networks, bioinformatics), energy optimisation (smart grids, resource allocation), machine learning (setting hyperparameters in hybrid models). For instance in production, a factory producing several types of product has to decide how much of each product to make to maximise its profit, while respecting the production capacity and market demand constraints. In this case, the quantities of products produced could be considered as continuous variables and decisions to switch certain machines on or off could be integer variables. More formally, the goal is to minimize (or maximize) a function f defined on d discrete and c continuous variables $(d, c > 0)$. Furthermore, in most real-world applications, the function f is not defined analytically and is often the result of numerical simulations, which makes it impossible to use the derivative. As a consequence, free-derivative methods as metaheuristics or Artificial Evolution (AE) (Del Ser et al. 2019) may be used (Ploskas and Sahinidis 2022). AE are nature-inspired and stochastic algorithms that mimic Darwin's theory for problem optimisation[1] by evolving a set of candidate solutions in silicio using selection, mutation, crossover and reproduction operators.

According to (Talbi 2024), MIO techniques can be divided into two different approaches: *global* or *decomposition-based*. In the *global* approach, the optimisation process is performed on the entire mixed variable space by considering the discrete variables as continuous variables, or discretising continuous variables. In the opposite, the *decomposition-based* approach involves optimising separately the continuous variables from the discrete ones. In this case, a *collaboration* strategy gives good performances. It decomposed the initial problem into several sub-problems, each of which is solved in a separate process to generate partial optimal solutions. All search processes collaborate together to construct complete solutions to the initial problem. Most of techniques in the literature studied by (Talbi 2024) mainly considers population-based metaheuristics for optimising both continuous and discrete variables. Some hybrid approaches combining global and decomposition-based approaches are mentioned, but most are based on a single AE technique such as DE, PSO or ACO... In most cases, the algorithm, initially dedicated to continuous optimisation is then adapted to deal with discrete variables.

Research questions. In this work, we believe that machine learning, and more specifically reinforcement learning (RL) with the Monte Carlo Tree Search (MCTS) algorithm (Świechowski et al. 2023; Browne et al. 2012), should give better results as it is well suited to combinatorial optimisation. It has been combined with deep learning (DL) to beat the world champion at Go (Silver et al. 2016). MCTS uses a policy to balance exploration and exploitation when selecting the most interesting state in the search space. (Sabharwal et al. 2012) initiated this approach by combining the upper confidence bound for trees (UCT) with CPLEX solvers. The basic idea is to hybridise MCTS with AE, since MCTS has proven its superiority for combinatorial optimisation and AE for continuous optimisation. In addition, both techniques have been adapted for the other type of optimisation. So which combination is better for MIO? As we have recently improved the MCTS algorithm in continuous space (Michelucci et al. 2024), we wonder which AE technique should be replaced by the MCTS approach ? It may also be possible to consider MCTS for both discrete and continuous optimisation, and as far as we know this has not been investigated.

Methodology and Work Plan. This PhD proposal is ambitious because it mixes two different subfields of computer science such as stochastic optimisation with artificial evolution and reinforcement learning with MCTS. The PhD work could be divided into the following phases:

[1] https://youtu.be/_Hj9fxMxBX0.

1. starting by developing an AE technique applied to MIO and comparing the results for the different approaches (global and decomposition-based) on benchmark functions;
2. based on the MCTS4R software library developed at the I3S laboratory for educational purposes, perform the same experimental protocol as in the previous step using the MCTS technique. Is it better to use the *global* approach with MCTS or the *collaboration* approach by combining vanilla MCTS with continuous MCTS? We have already developed a continuous version of MCTS in a bioinformatics context (Michelucci et al. 2024), but it should be generalised for other domains. Then, what about a nested approach to MCTS, considering both discrete and continuous variables in the same tree and using a different policy depending on the nature of the variable;
3. According to the results obtained in the previous steps, we will investigate different hybridisation strategies between AE and MCTS techniques for MIO. As presented above, we could envisage a collaboration between two sub-processes, one for discrete variables optimised with MCTS and another for continuous variables optimised with the AE technique. One could also envisage exploring the discrete variable space using MCTS by considering the transition between states as fixing a value for the selected discrete variable. A simulation would only be possible if all discrete variables were involved. The simulation would consist of optimising the continuous variables using an AE technique within a given budget.

Application domain. We first expect to test and compare our approaches on benchmark functions (Tušar et al. 2019) or from the library of mixed-integer and continuous nonlinear programming instances[2]. We then expect to validate our proposed algorithms to the field of bioinformatics and in particular to the modelling of Gene Regulatory Networks (GRNs). A regulatory network, modelled as a graph, defines the static interactions of a biological system. Each interaction abstracts the individual influence of a gene x on the expression of another gene y. The dynamics of the network are governed by a large number of discrete and continuous unknown parameters, which we aim to identify (Grataloup et al. 2024).

References

Browne, C. B., E. Powley, D. Whitehouse, S. M. Lucas, P. I. Cowling, P. Rohlfshagen, S. Tavener, D. Perez, S. Samothrakis, and S. Colton (2012). "A Survey of Monte Carlo Tree Search Methods". In: *IEEE Transactions on Computational Intelligence and AI in Games*. DOI: 10.1109/TCIAIG.2012.2186810.

Del Ser, J., E. Osaba, D. Molina, X.-S. Yang, S. Salcedo-Sanz, D. Camacho, S. Das, P. N. Suganthan, C. A. Coello Coello, and F. Herrera (2019). "Bio-Inspired Computation: Where We Stand and What's Next". In: *Swarm and Evolutionary Computation*. DOI: 10.1016/j.swevo.2019.04.008.

Grataloup, G., **D. Pallez**, G. Bernot, and J.-P. Comet (2024). "Single-Objective Constrained Optimization for Gene Regulatory Networks Modeling". In: *Artificial Evolution*.

Michelucci, R., **D. Pallez**, T. Cazenave, and J.-P. Comet (2024). "Improving Continuous Monte Carlo Tree Search for Identifying Parameters in Hybrid Gene Regulatory Networks". In: *PPSN*. DOI: 10.1007/978-3-031-70085-9_20.

Ploskas, N. and N. V. Sahinidis (2022). "Review and comparison of algorithms and software for mixed-integer derivative-free optimization". In: *Journal of Global Optimization*. DOI: 10.1007/s10898-021-01085-0.

Sabharwal, A., H. Samulowitz, and C. Reddy (2012). "Guiding Combinatorial Optimization with UCT". In: *Integration of AI and OR Techniques in Contraint Programming for Combinatorial Optimzation Problems*. DOI: 10.1007/978-3-642-29828-8_23.

Silver, D. et al. (2016). "Mastering the Game of Go with Deep Neural Networks and Tree Search". In: *Nature*. DOI: 10.1038/nature16961.

Świechowski, M., K. Godlewski, B. Sawicki, and J. Mańdziuk (2023). "Monte Carlo Tree Search: A Review of Recent Modifications and Applications". In: *Artificial Intelligence Review*. DOI: 10.1007/s10462-022-10228-y.

Talbi, E.-G. (2024). "Metaheuristics for variable-size mixed optimization problems: A unified taxonomy and survey". In: *Swarm and Evolutionary Computation*. DOI: https://doi.org/10.1016/j.swevo.2024.101642.

Tušar, T., D. Brockhoff, and N. Hansen (2019). "Mixed-integer benchmark problems for single- and bi-objective optimization". In: GECCO '19. DOI: 10.1145/3321707.3321868.

[2]https://www.minlplib.org