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Multivariate metaheuristics in nonlinear energy systems modelling: application to the optimal hydrogen supply chain design

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Abstract

The pathway towards net-zero emissions requires substantial infrastructure changes to allow the current energy system to provide the same level of services as of today, but with limited impact to global warming. The greenfield design of complex energy infrastructures is typically tackled as an optimization problem solved with mathematical programming, based on a Linear Programming (LP) or a Mixed-Integer Linear Programming (MILP) formulation. The common approach to reduce the problem to LP or MILP often involves the linearization or piece-wise linearization of nonlinear functions and constraints. However, in some cases the approximation of the problem would require the introduction of a large number of auxiliary variables to, e.g., avoid bi-linearities. When nonlinearities are kept in the problem formulation (MINLP problem) the problem can be computationally challenging even for small scales of application, and no single algorithm emerges as a clear winner. Overall, the methods for the solution of a MINLP problem can be classified in two groups: (i) based on a single design point in the decision variables space, like descent direction methods, and (ii) population methods based on a collection of design points, like metaheuristic algorithms. Among the latter, a specific class has been proposed to allow an abstract representation of the optimisation problem, in analogy to the state-of-the-art solvers in mathematical programming: multivariate metaheuristics. Within the field of energy system design, in the authors apply a multivariate metaheuristic method in an economic dispatch problem for the operation of the electrical power system. The problem includes a non-smooth and piece-wise function affected by the valve-point operation and the presence of prohibited zones. Other works apply this class of algorithms to a building optimization problem or the sizing of a hybrid photovoltaic-wind energy system. For the optimization of hydrogen supply chain design (HSCD), multiple works have already used metaheuristic algorithms, despite none is part of the class of multivariate metaheuristics. As an example, the authors of propose the non-dominated sorting genetic algorithm (NSGA-II) for the solution of the multi-objective HSCD under demand uncertainty.

This work is based on a two-stage hybrid optimisation algorithm integrating a multivariate metaheuristic with mathematical programming. The first stage computes the installed capacity of the production technologies, the output flows and the pressures of the network subject to the nonlinearities, while the second stage identifies the optimal flow and the installed capacities of the transport technologies. The comparison with a mixed-integer model solved with mathematical programming highlights the impact of the piece-wise approximations on the objective function and compares the respective computational costs for different sizes of the problem. The first part of the work focuses on the selection of one algorithm within the multivariate class, derived from different metaheuristics: Ant Colony Optimization (ACO-MV), Particle Swarm Optimization (PSO-MV), Differential Evolution (DE-MV), Adaptive Estimation Distribution Algorithm (AEDA-MV) and Genetic Algorithm (GA-MV). The second part of the work analyses the application of the selected algorithm to the optimization of the HSCD problem with nonlinearities. The analysis is based on the comparison of the MINLP model with the respective MILP model in which the nonlinearities are linearized with a coarse (1 break-point) and a refined (101 breakpoints) piece-wise affine approximation. Four nonlinearities are considered: (i) capex and (ii) efficiency functions of the electrolyzer, (iii) cost of conditioning associated to the gas compression from the production node to the network input and (iv) the Weymouth equation which defines the pressure drops between two nodes of the transport network due to the friction of the pipelines. The case study is based on the estimated hydrogen demand and availability of electricity per geographical node with a spatial granularity at the NUTS2 level.

The comparison of the metaheuristics shows that all the algorithms, apart from GA-MV, achieve the global minimum with negligible scatter among the solutions. PSO-MV presents the highest increase in the quality of the solution in the first iterations, while DE-MV the smallest. However, the first metaheuristic achieving an approximation of the global optimum is ACO-MV, which was selected for the second part of the analysis. By taking the solution of the refined MILP model as reference case, the coarse piece-wise linearization introduces a negligible relative error in the total cost of the system of $1.37 \cdot 10^{-7}$, $2.82 \cdot 10^{-5}$ and $5.64 \cdot 10^{-4}$ for the case of 5, 14 and 25 nodes respectively. The MINLP model with nonlinear capex and efficiency leads instead to a relative error of $1.25 \cdot 10^{-3}$, $7.19 \cdot 10^{-4}$ and $8.50 \cdot 10^{-4}$for the case of 5, 14 and 25 nodes respectively. The MINLP model with pressure drops and conditioning cannot be directly compared with the other models, but it leads to a further increase in the objective function of $2.50 \cdot 10^{-4}$, $7.78 \cdot 10^{-3}$ and $2.98 \cdot 10^{-2}$ relative to the MINLP model with only nonlinear capex and efficiency. The associated computational time is of different order of magnitudes when the metaheuristic is used and when not. The solution of the refined MILP model requires 0.16 s, 0.83 s and 1.88 s, while the solution of the MINLP problem with all the nonlinearities requires mostly 16 min, 2 h 54 min and 9 h 42 min for the case of 5, 14 and 25 nodes respectively. In terms of impact on the design of the system, a comparison can be done by considering the largest capacity installed in each geographical scale. Compared to the refined MILP model, the coarse MILP model and the MINLP model lead to a smaller installed capacity with a maximum impact of 0.25% for 5, 14 and 25 nodes. The associated impact on the capex is negligible for the coarse MILP and around $33.5 \cdot 10^3$ EUR for the case of 14 and 25 nodes.

Overall, the comparison of the best performing multivariate metaheuristic ACO-MV for the solution of the MINLP version of the HSCD problem with the MILP approximations of the same problem reveals that the algorithm is capable of finding good approximations of the global optimum, while handling nonlinear constraints. The comparison of the associated computational cost reveals that the metaheuristic algorithm should only be used when the inclusion of nonlinearities is strictly necessary. In this work, it is the case for the inclusion of the Weymouth equation as nonlinear constraint which was required to design the pressure levels of the transport network. Concerning the impact on the design variables of the problem, the introduction of the nonlinearities in the capex and in the efficiency only partially affects the capacity installed and the associated capex. In this case study, the maximum impact on the size of the installed capacities was found to be in the order of kW, limiting the relevance of considering the nonlinearities in capex and efficiency in case studies of small geographical scale of analysis.

Keywords: Multivariate Metaheuristics; Hybrid Optimisation; MINLP; Hydrogen supply chain.