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ABSTRACTS

Bin packing problem with scenarios

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The scenario based scheduling is one of the latest approaches in modeling scheduling problems including uncertainty. In this model, every job is assigned to one or more scenarios and only the jobs of one scenario are realized. However, this chosen scenario is unknown in the time of scheduling, so the algorithms have to consider each scenario.

We introduce a similar model to the bin packing problem which is the dual problem of scheduling. We have a set of items with sizes between 0 and 1, and every item is assigned to one or more scenarios. The items have to be packed into bins such, that for any scenario, the summarized size of items in this scenario is at most 1 in every bin.

The objective function of the standard bin packing problem is to minimize the number of bins. We show some extensions of this objective to the scenario based model. One can consider the scenario with maximal number of bins, or try to minimize the sum of the bins in the scenarios. The objective function can be defined as the number of bins used for all the scenarios. We also introduce a multi-objective optimization model regarding the scenarios as the simultaneously optimized objective functions.

We describe the scenario based bin packing problem with the different objectives, and we show some competitive analysis of the standard bin packing algorithms adapted for scenarios.

The formalization of a multi-objective optimization problem for molecular design

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The aim of molecular design is to find the structure with the desired properties, as some properties need to be maximized, or minimized or need to be close to the given targets. We incorporate these conflicting targets into a set of utility functions and apply multi-objective genetic algorithm to generate the set of Pareto optimal solutions.

The genes of the chromosomes represent the molecular fragments, while the originally huge chemical search space is conveniently described by the Joback estimation method. For the satisfaction of the design task property constraints can be defined, while targets are defined in the utility functions. The structural constraints of the molecule can be conveniently described by the relational constraints, these are the number of available groups (fragments) and their relation to each other defined by the octet rule and further equations. The modification of the multi-objective Non-dominated Sorting Genetic Algorithm-II (NSGA-II) was carried out for the testing of the proposed methodology, and novel genetic operators were also introduced to ensure reliable structures.

The efficiency of the defined formalization is tested on several benchmark problems, as the search for compounds having desired physical and chemical properties is an essential, yet complex problem in chemical, petrochemical and pharmaceutical industry.