set of 1125 CVRP instances. Using an online instance space analysis tool known as MATILDA, the instance space is visualized using selected features to reveal the diversity of the test instances, and the strengths and weaknesses of different algorithms. Finally, machine learning tools and techniques are used to predict the performance of algorithms to achieve an automated algorithm selection.

4 - The family traveling salesman problem with incompatibility constraints
Raquel Bernardino, Ana Paias

Consider a depot and a partition of the set of nodes into subsets, called families. The objective of the family traveling salesman problem (FTSP) is to find the minimum cost route that starts and ends at the depot and visits a given number of nodes per family. We propose a new variant of the FTSP by introducing incompatibilities between the families, that is, incompatible families cannot be visited in the same route. Thus, the FTSP with incompatibility constraints (FTSP-IC) consists of determining the minimum cost set of routes that begins and ends at the depot; visits a given number of cities in each family; and does not visit incompatible nodes in the same route. We propose compact and non-compact formulations for the FTSP-IC, which model the incompatibility constraints for each family implicitly in the compatibility graph. We also present a new set of valid inequalities. To evaluate the different models, we used the benchmark instances for the FTSP and generated incompatibility matrices. The computational experiment shows that the non-compact models outperform the compact ones. As the exact methods are unable to address the largest sized instances, we developed an iterated local search, which efficiently obtains solutions with a lower value than the branch-and-cut algorithm for most of the instances with an unknown optimal value.

■ MB-36

Monday, 10:30-12:00 - Virtual Room 36

Performance Assessment and Benchmarking

Stream: Multiobjective Combinatorial Optimization
Invited session
Chair: *Andreia Guerreiro*

1 - Techniques to analyze the anytime behavior of algorithms for multi-objective optimization
Alexandre D. Jesus, Luis Paquete, Arnaud Liefooghe, Bilel Derbel

In multi-objective combinatorial optimization it is often not possible to find the efficient set in a reasonable amount of time. As such, anytime algorithms are of particular interest since they allow a decision maker to trade off execution time with solution quality. However, analyzing their anytime behavior, which can be described in terms of a function of solution quality with respect to execution time, is not trivial. In particular, there are two main issues: (i) how to summarize the anytime behavior of an algorithm over multiple runs and/or problem instances; and (ii) how to compare algorithms and make decisions on which algorithm is better, when no algorithm outperforms the others at all times. In this talk we present techniques to build performance profiles that characterize the anytime behavior of an algorithm over different runs or problem instances, and to measure the quality of a performance profile as a scalar value. To demonstrate the practical usefulness of these techniques, we will showcase their application in comparing and automatically selecting algorithms for multi-objective combinatorial optimization problems. Finally, we present a new package for R that implements these techniques and provides a simple interface to use them for the analysis of anytime behavior.

2 - Recent Advances on the Computation of the Hypervolume Subset Selection Problem
Andreia Guerreiro, Vasco Manquinho, José Rui Figueira

Assessing the quality of outcome sets of approximation algorithms for multiobjective optimization is not trivial. Set-quality indicators, which map the image of a set of solutions (a point set) into a scalar value, are a convenient way to do this assessment. These may comprise, in a scalar, the proximity of the set of points to the Pareto front, as well as information regarding the distribution of points in the set. Performance assessment through quality indicators can be viewed as a transformation of the multiobjective optimization problem into a single-objective one, where the goal is to find a point set, frequently of bounded in size, that maximizes the quality indicator. Consequently, each indicator is biased towards some point sets, and some distributions. It is therefore important to understand such biases, in particular, to characterize indicator-optimal subsets.

The hypervolume indicator is one of the most widely used quality indicators due to its desirable theoretical properties. For example, the indicator-optimal subsets are subsets of the Pareto front, and theoretical results on the distribution of points in these subsets are known for the two-objective case. Already for the three-objective case this characterization rely mostly on the empirical approximations of the optimal subsets as the practical use of current algorithms is limited. This work discusses new advances on the computation of the hypervolume subset selection problem for 3 and more objectives.

■ MB-37

Monday, 10:30-12:00 - Virtual Room 37

Graphs, networks and nets in Bioinformatics

Stream: OR in Computational Biology, Bioinformatics and Medicine
Invited session
Chair: *Agnieszka Rybarczyk*

1 - Smart and Interpretable Neural Networks for Classification Learning in Bioinformatics
Thomas Villmann, Marika Kaden

Classification learning currently is dominated by the use of deep neural networks. Yet, these networks usually require a huge amount of data. Further, after training the network decision in the inference phase frequently is difficult to explain. We provide smart and interpretable networks based on prototype learning, which are easy to interpret and, importantly, are proven to be robust. In combination with intelligent data preprocessing the integrating of domain knowledge is possible by appropriate similarity measures like correlations, kernels or information theoretic measures for data discrimination. According to this domain knowledge integration these networks show performances comparable to deep networks while requiring significantly less training data and computational resources. In particular, we present variants of learning vector quantization. Starting from the basic model introduced T. Kohonen, we consider modifications of the basic model such as probabilistic variants as well as adaptive feature waiting, which explicitly offers insights regarding the decision process to the applicants. Further, these models allow an easy to integrate reject option to achieve high classification confidence and model certainty. This option is obtained by the evaluation of the hypothesis margin, implicitly optimized during the classification learning process. We illustrate the approach for application in medical diagnosis support as well as for biomolecular sequence processing.

2 - Structural identification of metabolites from MS/MS spectra by molecular graphs
Piotr Wawrzyniak, Piotr Formanowicz

Disease pathogenesis, drug discovery, response to the treatment - analysis of all of them requires identifying metabolites, small chemical compounds being a product of metabolism. Unfortunately, today only