

individuals into a minimum number of deletion areas, and we provide a MIP formulation to exactly solve real instances of the PLOHP containing up to 9.000 individuals and 3000 SNPs.

Session 3: *Algorithms for Multiobjective Sequence Alignment* – Luís Paquete, Maryam Abbasi, Miguel Monsanto, Pedro Matias

In this work, the multiobjective formulation of the pairwise sequence alignment problem is introduced, where a vector score function takes into account the substitution score and indels or gaps separately. Two solution methods are introduced: a multiobjective dynamic programming that extends classical algorithms for this problem and an epsilon-constraint algorithm that solves a series of constrained sequence alignment problems. A state pruning technique based on the concept of bound sets is also presented. Finally, its application to phylogenetic tree construction is discussed.

Session 4: *Genetic Programming Applied to Pharmacokinetics* – Sara Silva, Leonardo Vanneschi

Genetic Programming (GP) is the youngest paradigm inside the artificial intelligence research area called evolutionary computation, inspired by Darwinian evolution and Mendelian genetics. It consists on the automated learning of computer programs and, theoretically, it can solve any problem whose candidate solutions can be measured and compared. GP has been successfully used in many different application domains, and often yields results that are not merely academically interesting, but competitive with the work developed by humans. However, for two decades GP has suffered from the bloat problem, which consists on excessive code growth without a significant improvement in fitness, and it also suffers from the well known problem of overfitting. In this presentation we explain how GP can be applied to pharmacokinetics. In particular, we show the results of predicting the human oral bioavailability of medical drugs based on their molecular structure. We use the newest techniques to prevent bloat and we assess the improvements achieved while observing their (unexpected) effect on overfitting.

Session 5: *Optimization for some Open Problems in Chemoinformatics and Bioinformatics* – André O. Falcão

Optimization is a regular issue in many problems in bioinformatics and chemoinformatics. In bioinformatics, some of the central issues in protein function prediction are still being solved by brute force solutions in the search for optimal protein conformations. Yet even well known procedures like sequence alignment require optimization techniques for approximation to the best possible solutions. Chemoinformatics, despite