

Title: Multi-objective optimization in bioinformatics and computational biology

Abstract: Numerous problems encountered in bioinformatics and computational biology can be formulated as optimization problems and, thus, lend themselves to the application of meta-heuristic optimizers. Traditionally, the optimization is conducted with respect to a single goal. For certain applications a multi-objective formulation of the problem will offer concrete advantages, and thus introduce the need for the use of multi-objective optimization tools. The potential benefits of such an approach have now been demonstrated in various problems in computational biology ranging from classification problems, over model inference problems to protein structure prediction.

In this talk, I will provide an overview of the different conceptual reasons that can necessitate the use of multiple objectives, and underpin this discussion with concrete examples from computational biology. I then highlight two relevant areas from my own research, specifically the development and application of multi-objective clustering approaches, and investigations into the multi-objective formulation of the problem of de novo protein structure prediction.

References:

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- 2) J Handl, DB Kell, J Knowles (2007), Multiobjective optimization in bioinformatics and computational biology, *IEEE/ACM Transactions on Computational Biology and Bioinformatics* 4 (2), 279-292
- 3) J Handl, J Knowles, R Vernon, D Baker, SC Lovell (2012), The dual role of fragments in fragment-assembly methods for de novo protein structure prediction, *Proteins: Structure, Function, and Bioinformatics* 80 (2), 490-504