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Virtual BSC RS/Life Session: Global non-convex optimisation by Polynomial Model Based Optimisation (PMBO) for Tumor Response Models

Objectives

Abstract: We address global non-convex optimisation tasks by a novel approach given by modelling the expected improvement acquisition function by a polynomial. In contrast to classic Bayesian optimisation the method allows to follow analytic gradient descents identifying potential candidates of "optimal" samples. The approach is applied to a Tumor Response Model developed at the Valencia Lab, Life Science Department, BSC, demanding such a black box optimisation. As empirical results suggest the PMBO algorithm can identify optimal balance if Injection freunde, dose, and duration with much less simulation effort. The approach is intended to be extended to more (higher dimensional) complex optimisation tasks in this regard.



Short bio: Michael

is a mathematician with various interests reaching from the study of topological invariants of Hamiltonian systems to graph theoretical aspects of bioinformatics, approximation theory, numerical PDE solvers and regularisation techniques for machine learning methods. Michael leads a research group at CASUS - Center for Advanced Systems

Understanding, Goerlitz, Germany, realising algorithms that aim to lift the curse of dimensionality from multivariate interpolation, regression, and numerical integration tasks. Further, solutions for global optimisation, fast PDE solvers, level-set methods and beyond are developed. Thereby, the theoretical investigations aim to directly contribute freeing current challenges across scientific disciplines from their computational limitations, e.g., biophysical cell modelling, air pollution forecasting or HPC simulations for radiation physics.

Speakers

Speaker: Dr. Michael Hecht, Group Leader at CASUS - Center for Advanced Systems Understanding (Goerlitz, Germany)

Host: Alfonso Valencia, BSC Life Sciences department director

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

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