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Pod Vodárenskou věží 2, Praha 8 - Libeň
konat přednáška

Knowledge discovery for black-box optimization

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Abstract: The term "black-box optimization" refers to optimization of functions without knowing their mathematical expression (neither an explicit one, as a composition of known functions, nor an implicit one, as a solution of explicitly stated equations). Values of black-ox functions can be obtained only empirically, through measurements or simulations. Most successful in black-box optimization are evolutionary algorithms, due to weak assumptions about the optimized function (which is in the evolutionary context usually called fitness). However, working only with function values of the fitness, an evolutionary algorithm needs a large number of its evaluations, which causes problems in situations when the empirical evaluation of the black-box fitness is time-consuming and/or costly. As a remedy, data mining has been used for approximately 15 years, applied to data from the previous generations of the evolutionary algorithm. It yields a regression model approximating of the black-box fitness, a.k.a. its surrogate model, which is used instead of the original fitness in a substantiv part of its evaluations. The talk will attempt to illustrate both the theoretical research in surrogate modelling for evolutionary optimizition, by Lukáš Bajer, Zbyněk Pitra, Jakub Repický and myself, and its applicability to real-world problems. In the theoretical context, it will present surrogate modelling primarily in connection with the state-of-the-art evolutionary algorithm for black-box optimization, the covariance matrix adaptation evolution strategy. It will concentrate on the most sophisticated among the encountered surrogated models, Gaussian processes, though it will briefly sketch also random forests and models based on various kinds of articial neural networks. As a real-world application, the talk will show how evolutionary optimization and its extension with surrogate models are used to optimize catalysts for given chemical reactions.