Vitalii Zankin (Skoltech, Moscow), Gradient Descent Approach to the Experimental Design with Application to Multivariate Function Approximation,

Abstract:

Many processes and systems in various fields of science and technology are emulated by using computational models. However, in many cases, these models turn out to be so computationally costly that, for example, their optimization over the values of input parameters turns out to be prohibitively expensive or even impossible. One of the approaches to solve such problems is surrogate modeling that is an approximate polynomial expansion over a certain basis. To find the coefficients of such an expansion, the least-squares method is usually used. This method allows to calculate the expansion coefficients of the approximate model for a fixed number of evaluations of the initial computational model. However, the quality of the approximate model constructed in this way essentially depends on the choice of the values of input parameters at which the initial computational model is evaluated. Thus, the problem of so-called Design of Experiments arises. In order to solve it, it is needed to develop a method for selecting such values of the input parameters of a computational model for which the polynomial approximation obtained by the least-squares method will have as small approximation error as possible. In this work, we propose a new method for Design of Experiments. This method allows to sample such input values of the parameters of a computational model for which the constructed approximate model will have the least possible approximation error. High efficiency of proposed method is demonstrated by its comparison with other sampling methods (LHS, Sobol? sequence sampling, and Maxvol sampling) on the problem of multivariate function approximation. Also, numerical experiments for the Lebesgue constant growth for the points sampled by the proposed method are carried out.