Optimal Experimental Design in Chromatography

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Abstract

We study Bayesian optimal experimental design in a Chromatography process. The mathematical model is governed by a non-linear hyperbolic PDE which depend of 4 unknown parameters and the 2 design variables: the time injection and the amount of concentration. The quality in the inversion process depends of the selection of the design variables and the number of nodes for measurements. The algorithms used for estimate the utility function are based in Monte Carlo estimations, and a surrogate model based in piecewise linear interpolation over sparse grids. The results conclude independence respect to the time injection for huge quantity of measurement nodes and periodicity for few nodes.