Abstract

We investigate optimal design strategies for discriminating between candidate models. The goal is to consider and develop design strategies to cover both cases of standard design theory with independent observations and the design issue in the context of correlated observations. The latter has been rarely considered in the literature specifically in the discriminating experiments.

We first compare the performances of sequential design algorithms for discrimination of enzyme kinetic models. Three design strategies are considered. One of the design approaches (δ-optimality) is extended to a sequential version, while others require adjustments for the specific enzyme kinetic models. Another issue considers a change of assumption in the error structure of the considered enzyme kinetic profiles by assuming multiplicative lognormal errors. We observe that the logarithmic transformation of models decisively affects the optimal designs and their efficiencies.

Investigation of design criteria to discriminate between Gaussian process models is another main focus. We look attentively at different modes of design construction for model discrimination, develop and present the corresponding design criteria. Availability of the observations corresponding to previously constructed design points makes a distinction in construction of criteria in prediction-based mode. Multiple static design criteria are considered in distance-based mode including the familiar log-likelihood ratios and the Fréchet distance between the covariance functions. A novel family of criteria is introduced which is simpler to calculate compared to the rest. These novel criteria have the property to extend to a design measure version. A necessary condition for optimality of such designs is developed in a theorem. A simplified problem with an explicit optimal solution is provided in another theorem followed by subsequent discussions.

Numerical examples and simulation studies demonstrate design implications, allow comparisons and illustrate theoretical results.