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Bayesian optimal designs for the Michaelis-Menten Model

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The Michaelis-Menten model describes the velocity rate in many enzymatic reactions. This model is used in cases when the concentration of the substrate is higher than enzyme concentration, and when the concentration of the substrate-enzyme compound stays constant. Biochemical reactions involving a single substrate are also often modelled with this equation. Using the optimal experiment design theory for non-linear regression models, like the Michaelis-Menten model (e.g. [3, 4, 5], we have applied the D-optimal criteria and the pseudo Bayesian D-optimal criteria and found the optimal design for each case. The so called General Equivalence Theorem provides a fantastic tool for checking whether a particular design is optimal or not with respect to a convex criterion. When applying Bayesian optimality (e.g. [1, 2]) a closed-form expression for the optimal design is not always available for this model. Therefore, numerical computations have performed for different cases. Two different Bayesian approaches have been used. On the one hand the expectation of any criterion according to the prior distribution has been used. This is sometimes called pseudo-Bayesian and it is very much used in the literature. A more sophisticated version considers an information matrix which depends on the sample size and the prior covariance matrix. We have compared different optimal designs for both approaches and different values of the sample size. Adapted equivalence theorems allow for computation and measuring the efficiency of the designs obtained. Keywords: Bayesian Optimal Designs; D-optimality; Equivalence Theorem; Fisher Information Matrix.

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