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Optimum Designs for Enzyme Inhibition Models: Algorithmic Approach.

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SUMMARY

Enzyme kinetics study the rate of substrate that are transformed into products during a reaction catalyzed by an enzyme [1]. The characterization of these processes is of wide interest for the correct interpretation of the chemical mechanisms that take place during a chemical reaction.

An experimental design consists of a planned collection of points in a given space $\mathcal{S}\times\mathcal{I}$ where experimental observations are taken. In this work, the design criteria used are $D-$ and $A-$optimality. The $D-$optimal criterion minimizes the volume of the confidence ellipsoid of the parameters and is given by $\phi_D[M(\xi;\theta)] = \det M(\xi;\theta)^{-1/k}$, where k is the number of parameters in the model. The A-optimal criterion minimizes the sum of the variances of the parameters and is given by $\phi_A[M(\xi;\theta)] = \text{tr } M(\xi;\theta)^{-1}$.

The Wynn-Fedorov algorithm to compute optimal designs used in this work adds a new point to an initial design based on the information provided by the Equivalence Theorem at each iteration [2]. Its application to multifactor models, as the proposed, shows the advantages and disadvantages of the algorithm.

Keywords: Optimum Designs, Enzyme Inhibition, Wynn-Fedorov Algorithm

AMS Classification: 62K05

References

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