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Building Pharmacokinetic Compartmental Models Using a Superstructure Approach

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Abstract

An optimization framework is presented to support the model builder in elucidating compartmental models that plausibly describe data obtained during experimentation. Here, one specifies a priori the maximum number of compartments and type of flows to contemplate during the optimization. The mathematical model follows a 'superstructure' approach, which inherently considers the different feasible flows between any pair of compartments. The model activates those flows/compartments that provide the optimal fit for a given set of experimental data. A regularized log-likelihood function is formulated as the performance metric. To deal with the resulting set of differential equations orthogonal collocation on finite elements is employed. A case study related to pharmacokinetics of an oncological agent demonstrates the advantages and limitations of the proposed approach. Numerical results show that the proposed approach can provide 33% smaller mean square prediction er-

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