Development of R-Package for Estimation of Stochastic Enzyme Kinetics Model

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Enzyme Kinetics Model is one of the major methods of studying chemical reactions by enzymes, mainly used in pharmaceutical research and food biotechnology. The method(Michaelis et al. 1913), which Michaelis-Menten suggested, of Enzyme Kinetics Model has been using world wide, and specifically, various approximation models are used depending on specific constraints. In this research, The Standard Quasi Steady State(sQ) model and Total Quasi Steady State(tQ) model are used to estimate the kinetic model of the enzyme reaction kinetics. Based on this, we tried to estimate the parameters through the Bayesian approach by extending the Stochastic Simulation Approximation (SSA) of R-package, EKMCMC(Choi et al, 2017) using the existing probabilistic approach to the parameter estimation for the enzyme kinetics model with three methods including Diffusion Approximation(DA) and Gaussian Process(GP). In addition, we developed an R package containing the above estimation process, so that analysts who have basic knowledge of R can obtain the results by setting the argument for the function embedded in the package to the researcher's objective without knowledge of the statistical procedure.

REFERENCE

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