Parameter Estimation for Physiologically Based Pharmacokinetic (PBPK) Model by Bayesian Inference

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Physiologically based pharmacokinetic(PBPK) model is mathematical technic for predicting absorption, degradation, execration and other metabolisms in drug delivery system. It is useful technic for regulating dose to prevent side effect of drug and observing drug concentration at a particular time during the clinical demonstration. Since PBPK model is expressed as simultaneous differential equation with various parameters, we need to solve non-linear differential equation and estimate parameters to predict concentration as a function of time at each organs. However, because experimental data of drug delivery system are noisy and sparse, it is difficult to estimate correct parameter value with non-linear regression. In this reason, we introduce Bayesian inference for parameter estimation of PBPK model. We demonstrate advantages of Bayesian inference compared with non-linear regression, conduct case study about Tegafur delivery system.