System identification of Sparse Stochastic Monomolecular Biological Reaction Networks

장 홍, 이재형*
한국과학기술원
(jayhlee@kaist.ac.kr*)

A sparse parameter estimation method is proposed for identifying a biochemical reaction network system. Identification of a reaction network can be achieved by estimating a sparse parameter matrix containing the reaction network structure and kinetics information. Stochastic dynamics of a biochemical reaction network system is usually modelled by a chemical master equation describing the time evolution of probability distributions for all possible states. This paper considers monomolecular reaction systems representing many biological systems for which an analytical solution of the corresponding chemical master equation is available. The estimation method presented in this paper incorporates the closed-form solution into a regularized maximum likelihood estimation (MLE) for which model complexity is penalized. A simulation study with 5 species reaction network system is tested to verify performance improvement of the presented regularized MLE over the least squares (LSE) based on a deterministic mass-average model in the case of a small population size.