System identification of metabolic networks using Nonlinear Bayesian filtering*

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Understanding dynamic behavior of metabolism is a major challenge in systems biology. To address this challenge, quantitative mathematical models are needed. The metabolite concentration in living cells can be described by complex systems of nonlinear differential equations with a relative large number of parameters. Nonlinear Bayesian filtering is an approach that allows simultaneous estimation of parameters and states of the underlying system. Various methods of this kind, such as the Extended Kalman Filter, the Unscented Kalman Filter and the Particle Filter have been proven useful in many applications of science and engineering.

Our work compares nonlinear Bayesian tools for simultaneous estimation of parameters and states in metabolic networks. The first step towards applying the above methods to real data was to develop an unified framework and set up a simulation environment for systems biology data to evaluate the methods in a controlled environment. The methods were then compared using mean squared error statistics when applied to the synthetic network. It is concluded that this is a feasible approach to identify systems of such type.

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