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Adaptive Unscented Kalman Filter for Estimation of Parameters in Kinetic Metabolic Models

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1 Introduction

Parameter estimation is considered to be one of the greatest challenges in computational systems biology. Biological experiments can measure only a fraction of the kinetic parameters and the rest has to be estimated in silico. Recently parameter estimation problems have been addressed in the framework of control theory. One of the most successful and widely used methods in control theory for estimation of states and parameters is the Kalman filter and its various non linear extension like Extended Kalman Filter (EKF) and Unscented Kalman Filter (UKF). Lillacci et. al. [3] successfully applied EKF whereas Baker et. al. [1] applied UKF for parameter estimation in biological models. Though UKF has shown promising results in estimating unknown parameter value in biological models where the system is defined by nonlinear ODEs, it still inherits some of the limitations of Kalman Filter which means, it can achieve good results under prior assumptions of proper information of the noise distribution and proper initial conditions. But this a priori information is not always available in practice and so assumptions have to be made. If the assumptions are not correct, it might lead the filter to diverge from the solution. One way to solve the problem would be to introduce adaptive mechanism into normal UKF which will also estimate the parameters to match the real statistics and which are not known a priory. Zhe Jiang et. al. [2] proposed a novel adaptive UKF (AUKF) which could make nonlinear joint estimation of both time-varying states and error covariance statistics.

2 Method

In AUKF two parallel UKFs will be running. One will be called master UKF and the other slave UKF. The master UKF is used to estimate the states and parameters whereas the slave UKF estimates the diagonal elements of the noise covariance matrix for the

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master UKF. Slave UKf will do that based on innovations generated by the master UKF. Both the master and slave UKF's are independent of each other.

There are couple of parameters in UKF that can be tuned. Among those parameters a priori knowledge on process noise covariance matrix Q and measurement noise covariance matrix R are the most important for the performance of the accuracy of UKF [2]. If these two parameters are too low then the uncertainty tube will become low and if it is too high it might cause the divergence of the filter. In this paper we try to tune measurement noise covariance R by using AUKF. We could describe the measurement noie covariance matrix R by using θ_k^i in the diagonal of a matrix to denote the i^{th} diagonal element of this matrix R_v^k In this paper we have implemented AUKF for parameter estimation on model of upper part of Glycolysis from yeast. Set of ODEs are formulated from this case study model to formulate the mathematical model of the network. There are in total 15 parameters in the model and among those 15 parameters 4 parameters are estimated using AUKF.

Table 1 summarizes the statistics from 100 runs of each of the algorithms. The statistics clearly shows a better performance of AUKF over normal UKF. For AUKF the mean value reaches more closer to the actual value and also the standard deviation of the estimation is much lower compared to that of UKF. Specially the standard deviation for $V_{max,4}$ is quite high in UKF which is significantly minimized in AUKF. All these makes AUKF more precise and reliable.

Algorithm Name	Parameter Name	Mean	Standard Deviation	Average Actual Value
UKF	$v_{max,4}$	45.54	3.10	44.72
	K_2	2.38	0.28	2.26
	$v_{max,3}^f$	140.46	0.66	140.28
	K_{8r}	133.45	0.45	133.33
AUKF	$v_{max,4}$	44.72	0.15	44.72
	K_2	2.26	0.03	2.26
	$v_{max,3}^f$	140.42	0.59	140.28
	K_{8r}	133.30	0.41	133.33

Table 1: Results obtained by repeating the computation of UKF and AUKF in the case study model 100 times. Statistics of the data are calculated from this 100 runs.

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