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A maximum-likelihood method for estimating parameters, stochastic disturbance intensities and measurement noise variances in nonlinear dynamic models with process disturbances

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ABSTRACT

An improved approximate maximum likelihood algorithm is developed for estimating measurement noise variances along with model parameters and disturbance intensities in nonlinear stochastic differential equation (SDE) models. This algorithm uses a Laplace approximation and B-spline basis functions for approximating the likelihood function of the parameters given the measurements. The resulting Laplace approximation maximum likelihood estimation (LAMLE) algorithm is tested using a nonlinear continuous stirred tank reactor (CSTR) model. Estimation results for four model parameters, two process disturbance intensities and two measurement noise variances are obtained using LAMLE and are compared with results from two other maximum-likelihood-based methods, the continuous-time stochastic method (CTSM) of Kristensen and Madsen (2003) and the Fully Laplace Approximation Estimation Method (FLAEM) (Karimi and McAuley, 2014). Parameter estimations using 100 simulated data sets reveal that the LAMLE estimation results tend to be more precise and less biased than corresponding estimates obtained using CTSM and FLAEM.

1. Introduction

Fundamental models based on mass and energy balances are imperfect representations of process behavior due to simplifying assumptions and approximations that ignore complex interactions (Maria, 2004). Model uncertainties may also arise from random disturbances associated with feed streams and the environment of the chemical process (Gagnon and MacGregor, 1991; Srivastava et al., 2013). As a result, some modelers add stochastic terms to their dynamic fundamental models to account for model mismatch and process disturbances, resulting in systems of stochastic differential equations (SDEs) (King, 1974; Érdi and Tóth, 1989).

In this article, we consider a Multi-Input Multi-output (MIMO) nonlinear SDE model of the following form:

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\theta}) + \boldsymbol{\eta}(t) \tag{1.a}$$

$$\mathbf{x}(t_0) = \mathbf{x}_0 \tag{1.b}$$

$$\mathbf{y}(t_{mr,j}) = \mathbf{g}(\mathbf{x}(t_{mr,j}), \mathbf{u}(t_{mr,j}), \boldsymbol{\theta}) + \boldsymbol{\varepsilon}(t_{mr,j}) \tag{1.c}$$

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Nomenclature

Abbreviations

AEM	approximate expectation maximization
AMLE	approximate maximum likelihood estimation
CSTR	continuous stirred tank reactor
CTSM	continuous time stochastic modeling
EKF	extended Kalman filter
IQR	interquartile range
LA	Laplace approximation
LAMLE	Laplace approximation likelihood method
MCMC	Markov chain Monte Carlo
MIMO	multi-input multi-output
ML	maximum likelihood
MLE	maximum likelihood estimation
SDE	stochastic differential equation
SML	simulated maximum likelihood

Roman letters

a	CSTR model parameter relating heat-transfer coefficient to coolant flow rate
b	CSTR model exponent relating heat-transfer coefficient to coolant flow rate
c_s	number of B-spline coefficients for sth state trajectory
C_A	concentration of reactant A (kmol m^{-3})
C_{A0}	feed concentration of reactant A (kmol m^{-3})
c_p	heat capacity of reactor contents (J kg^{-1} K^{-1})
c_{pc}	coolant heat capacity (J kg^{-1} K^{-1})
C_1	constant in Eq. (15)
C_2	constant in Eq. (A.7)
C_3	constant in Eq. (B.6)
cov{.}	covariance
$\mathbf{D}$	function of $\mathbf{f}$ and its derivatives shown in Eq. (B.16)
det	determinant
dim	dimension of a vector
$E\{.\}$	expected value
E/R	activation energy divided by the ideal gas constant (K)
$\mathbf{f}$	X-dimensional nonlinear function on the right-hand side of the SDE model (Eq. (5))
F	reactant volumetric flow rate (m^3 min^{-1})
F_c	coolant volumetric flow rate (m^3 min^{-1})
$\mathbf{g}$	Y-dimensional vector of nonlinear functions on the right hand side of Eq. (5)
$\mathbf{G}$	derivative of J_1 defined in Eq. (B.29)
g_r	nonlinear function on the right hand side of Eq. (1.c) for rth measurement
ΔH_{rxn}	enthalpy of reaction (J kg^{-1} K^{-1})
$\boldsymbol{H}_{\mathbf{X}\sim}$	Hessian matrix of the $-\ln p(\mathbf{X_q}, \mathbf{Y_m}\vert\zeta)$ with respect to $\mathbf{X_q}$ evaluated at $\mathbf{X_{q\sim}}$
$\boldsymbol{H}_{\mathbf{B}}$	Hessian matrix of the $-\ln p(\mathbf{X_q}, \mathbf{Y_m}\vert\zeta)$ with respect to B-spline basis functions
$\mathbf{H}_{\mathbf{x_r}\sim}$	Hessian matrix defined in Eq. (C.3)
H_{β_r}	Hessian matrix defined in Eq. (C.7)
$\mathbf{I}$	identity matrix
j_1 and j_2	positive integers in Eq. (3)
$J_{AMLE,CSTR}$	AEM objective function for CSTR model defined in Eq. (25)
J_{AMLE}	AMLE objective function defined in Eq. (11)
J_1	objective function defined in Eq. (A.2)
J_d	objective function defined in Eq. (B.6)
k_{ref}	kinetic rate constant at temperature T_{ref} (min^{-1})
k_r	rate constant defined in Eq. (22)
M	order of B-spline basis functions
n	number of measurements
n_C	number of measurements for concentration of reactant A
N_r	number of measurements for rth response
n_T	number of measurements for temperature
P	number of unknown model parameters
$p(.)$	probability density function
q	number of discretization points for SDE model (Eq. (1))
$\mathbf{Q}$	diagonal power spectral density function