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Parameter Subset Selection in Differential Equation Models with Dead Time

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Abstract: A methodology is proposed for parameter ranking and parameter subset selection for nonlinear ordinary differential equation (ODE) models with time delay, in which delay is treated as an unknown model parameter. The methodology builds on earlier algorithms for ranking model parameters in systems without time delay (Yao et al., 2003; Thompson et al., 2009) and for finding the optimum number of parameters for estimation (Wu et al., 2011; McLean and McAuley, 2012a). A polymerization reactor system for producing bio-source polyether is used to illustrate the effectiveness of the proposed method in comparison with prior results obtained by Cui et al. (2015) who neglected the time delay.

Keywords: mathematical models, time-delay estimation, identifiability, parameter estimation, differential equations, nonlinear equations, algorithms

1. INTRODUCTION

Fundamental models are used for scale-up, control, and optimization of chemical processes. Obtaining accurate model predictions requires estimation of model parameters and often making decisions about which parameters should be estimated from available data and which should be fixed at reasonable values or removed via model simplification (Walter and Pronzato, 1997; Chu et al., 2009; McLean and McAuley, 2012a; Kravaris et al., 2013). Several algorithms have been developed to determine which parameters can and/or should be estimated. The most popular methods rely on forward-selection to rank the parameters from most estimable to least estimable (Yao et al., 2003; Lund and Foss, 2008; Thompson et al., 2009). A mean-squared-error selection criterion is then used to find an appropriate number of parameters to estimate to obtain reliable predictions (Wu et al., 2011; McLean et al., 2012b; Eghtesadi and McAuley, 2016). For example, Table 1 shows an orthogonalization-based parameter-ranking algorithm and Table 2 shows an algorithm for selecting parameters to obtain low mean-squared prediction errors.

Algorithms in Tables 1 and 2 and other related subset selection methods were developed for parameter selection in dynamic models without time delay (e.g., Chu et al., 2009). Sometimes, however, modelers need to account for significant delay. In situations, where delays are associated with measurements or with piping that is not part of a recycle stream, deadtime can be handled during parameter estimation either by shifting the experimental data backward in time or shifting the predictions forward. If the delay arises in an internal recycle stream, deadtime must be considered within the model (e.g., using delay differential equations).

The objective of this article is to show how algorithms in Tables 1 and 2 can be extended to rank parameters and select appropriate subsets for estimation when deadtime appears as an unknown model parameter. We use a polymerization system with unknown time delay and unknown mass hold-up due to an overhead condenser to illustrate the proposed methodology.

2. PROPOSED METHODOLOGY

Consider an ordinary differential equation (ODE) model with time delay of the form:

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta_m}) \tag{1a}$$

$$\boldsymbol{x}(t_0) = \boldsymbol{x_0} \tag{1b}$$

$$\boldsymbol{y}(t) = \boldsymbol{g_d}(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta_m}, \theta_d, t) + \boldsymbol{\varepsilon} \tag{1c}$$

where $\dot{\boldsymbol{x}}$ is a vector of state variables, t is time, $\boldsymbol{f}$ is a vector of non-linear functions, $\boldsymbol{u}$ is a vector of input variables, $\boldsymbol{\theta_m}$ is the vector of unknown model parameters that appear in the ODEs, $\boldsymbol{x_0}$ is a vector of initial conditions for the state variables, $\boldsymbol{y}$ is a vector of measured output variables (some of which are affected by an unknown time delay θ_d), $\boldsymbol{g_d}$ is a vector of model predictions that accounts for this time delay in the affected responses and $\boldsymbol{\varepsilon}$ is a vector of zero-mean random variables. For simplicity, the time delay θ_d does not influence any of the state variables within the ODEs in (1a), but the proposed methodology could be readily used for more complex systems with time delay in the state variables rather than simple additive delay.

In (1c) the delay influences some but not all of the outputs. For example, a prediction of the i^{th} delayed response is $\boldsymbol{g_{di}}(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta_m}, \theta_d, t) = \boldsymbol{g_i}(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta_m}, t - \theta_d)$ where $\boldsymbol{g_i}$ is the

nonlinear mapping that would apply for the i^{th} response if there were no delay in the system.

Table 1. Orthogonalization algorithm for ranking model parameters (Yao et al., 2003; Thompson et al., 2009)

1 Calculate the magnitude (i.e., the Euclidean norm) of each column in the scaled sensitivity matrix Z. The most estimable parameter corresponds to the column in Z with the largest magnitude. Set k = 1.

2 Put the k columns from Z that correspond to parameters that have been ranked into matrix X_k.

3 Use X_k to predict columns in Z using ordinary least-squares

$$\hat{Z}_k = X_k (X_k^T X_k)^{-1} X_k^T Z \quad (1.1)$$

and calculate the residual matrix

$$R_k = Z - \hat{Z}_k \quad (1.2)$$

4 Calculate the magnitude of each column in R_k. The $(k+1)^{th}$-most estimable parameter corresponds to the column in R_k with the largest magnitude.

5 Increase k by 1, and put the columns corresponding to the k + 1 parameters that have been ranked in matrix X_k.

6 Advance the iteration counter k and repeat Steps 3 to 5, until all parameters are ranked or it is impossible to perform the least-squares prediction of Z in Step 3 due to matrix singularity.

The parameter ranking algorithm in Table 1, which was developed for systems without time delay, relies on a scaled sensitivity matrix Z with *p* columns and *N* rows, where *p* is the number of model parameters and *N* is the number of data values available for parameter estimation. For example, consider a chemical reactor system where *d* different types of responses variables (e.g., *d* different composition variables) are measured *n* times each during *r* different dynamic experimental runs, then $N = dnr$. The element in the i^{th} row and j^{th} column of Z is:

$$\left.\frac{\partial g_i}{\partial \theta_{m,j}}\right|_{\boldsymbol{\theta}_m, k \neq j} \frac{s_{\theta_{m,j}}}{s_{y_i}}$$

where g_i is the prediction of the i^{th} data value, $i = 1 \ldots N$, $s_{\theta m,j}$ is a scaling factor accounting for the uncertainty in the initial guess for parameter $\theta_{m,j}$ and s_{yi} is a weighting factor that accounts for uncertainties in measurements associated with the i^{th} measured value (Thompson et al., 2009). The elements of Z are computed numerically by solving sensitivity equations or by using difference approximations involving perturbations in parameter values from their initial guesses. The prescribed scaling makes the elements of *Z* dimensionless so that Z^TZ is a Fisher information matrix. Each row in Z corresponds to a measured value that is available to estimate the parameters.

Table 2. Algorithm to find the Optimum Number of Parameters for Estimation (Wu et al., 2011; McLean and McAuley, 2012a)

1 Rank model parameters from most to least estimable using the orthogonalization algorithm in Table 1.

2 Use weighted least-squares regression to estimate the first parameter from the list, with all others fixed at initial guesses. Next, estimate the top two parameters, followed by the top three parameters and so on, until all the ranked parameters have been estimated. Denote the value of the objective function with the top k parameters estimated and the remaining (p–k) parameters held fixed as J_k. Weighting factors used in the objective function for parameter estimation should be consistent with measurement uncertainties s_{y_i} used for scaling during parameter ranking.

3 Compute the critical ratio

$$r_{C,k} = (J_k - J_p)/(p-k) \quad (2.1)$$

for k = 1... p – 1.

where J_k is the objective function when the top k parameters have been estimated.:

4 For each value of k, compute the corrected critical ratio

$$r_{CC,k} = \frac{p-k}{N}\left(r_{CKub,k} - 1\right) \quad (2.2)$$

where

$$r_{CKub,k} = \max\left(r_{C,k} - 1, \frac{2}{p-k+2} r_{C,k}\right) \quad (2.3)$$

5 Select the value of k corresponding to the lowest value of $r_{CC,k}$ as the appropriate number of parameters to estimate.

In the parameter ranking algorithm in Table 1, the first step is to calculate the magnitude of each column in *Z*. Columns with large magnitudes correspond to parameters that have large influence on the response variables, relative to their corresponding initial uncertainty. The parameter with the largest overall influence, which is ranked first by the algorithm, is the most estimable parameter. Steps 2 to 4 are used to account for and remove the effects of correlation among the parameters. Using this algorithm, influential parameters that are initially poorly known appear near the top of the ranked list, whereas unimportant parameters and parameters whose values are already well-known rank near the bottom.

In the proposed methodology, the un-delayed predictions are replaced by the corresponding delayed predictions in the Z matrix; As a result, the scaled sensitivity coefficients become:

$$\left.\frac{\partial g_{d\,i}}{\partial \theta_j}\right|_{\theta_{k\neq j}} \frac{s_{\theta_j}}{s_{y_i}}$$

where $\boldsymbol{\theta}$ is the vector of model parameters augmented by the time delay parameters.

$$\boldsymbol{\theta} = \begin{bmatrix} \boldsymbol{\theta_m} \\ \theta_d \end{bmatrix} \qquad (2)$$

In (2), only one time-delay parameter θ_d is shown for simplicity, but multiple time-delay parameters could be added to the parameter vector for systems with multiple unknown delays. The Z matrix corresponding to (2) contains an additional column, which contains scaled sensitivity coefficients with respect to with respect to θ_d. The corresponding column of sensitivities can be calculated using difference approximations:

$$\left.\frac{\partial g_{d\,i}}{\partial \theta_d}\right|_{\boldsymbol{\theta_m}} \frac{s_{\theta_d}}{s_{y_i}} = \left.\frac{\Delta g_{d\,i}}{\Delta \theta_d}\right|_{\boldsymbol{\theta_m}} \frac{s_{\theta_d}}{s_{y_i}} \qquad (3)$$

3. EXAMPLE

The system for polyether production from 1,3-propanediol shown in Fig. 1 is used to illustrate the proposed methodology. In this process, an initial amount of liquid monomer is added to the batch reactor and then catalyst is added to start the polymerization. As polymerization proceeds, water and oligomers are produced. Nitrogen gas is sparged into the reactor to assist with water removal so that high-molecular weight polyether can be produced. Water diffuses from the reaction mixture into the nitrogen bubbles, which carry water vapour (and also some volatile oligomers) into the reactor headspace. The overhead vapour flows to a condenser and the resulting liquid is collected and analysed. Time delay arises because of time spent by vapour and liquid in the piping that leads to and from the condenser. Experimental data are available from liquid samples of the reactor contents (un-delayed responses for 12 state variables) and for the liquid sampled at the entrance to the condensate collector (delayed responses for 8 state variables). Cui et al. (2015) developed an ODE model for the reactor system, neglecting the time delay and the dynamics associated with accumulation of liquid species in the condenser. They used the available data to select and estimate 15 of the 18 kinetic and mass-transfer parameters that appear in the ODEs. Unfortunately, poor fits were obtained for some of the data, presumably because the time delay and condenser hold-up had been neglected.

Table 3 shows additional model equations that we developed to describe the operation of the condenser system. ODEs (3.1) to (3.3) and (3.5) describe time-varying concentrations of water $[W]_c$, propanal $[AD]_c$, monomer $[L(1)]_c$ and volatile linear oligomers $[L(q)]_c$, q=2..5 (i.e., dimer to pentamer) in the condenser liquid that would correspond to the condensate concentration measurements if there were no delay. The first term on the right-hand side of (3.1) is the flow rate of water into the condenser liquid, where F_{gtot} is the total molar flowrate of overhead vapour from the reactor, L_f is the fraction of this vapour that condenses (determined from an instantaneous flash calculation) and x_W is the mole fraction of water in this liquid inflow stream.

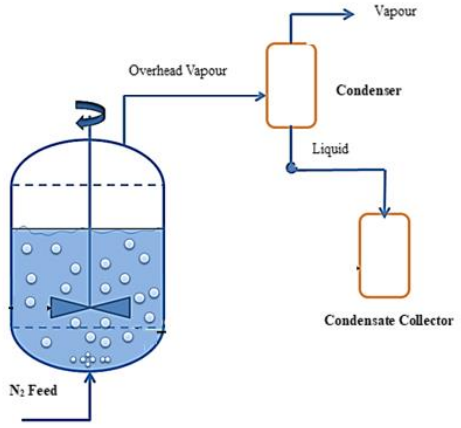

Fig. 1. PO3G reactor and condenser system (Cui et al., 2015)

Table 3. Differential equations for condenser and condensate collector

$\frac{d[W]_c}{dt} = \left(F_{gtot}L_f x_W - F_{gtot}L_f M_{L_f}[W_c]\right)\frac{1}{m_c}$	(3.1)
$\frac{d[AD]_c}{dt} = \left(F_{gtot}L_f x_{AD} - F_{gtot}L_f M_{L_f}[AD_c]\right)\frac{1}{m_c}$	(3.2)
$\frac{d[L(q)]_c}{dt} = \left(F_{gtot}L_f x_{L(q)} - F_{gtot}L_f M_{L_f}[L(q)_c]\right)\frac{1}{m_c}$	(3.3)
where q = 1, 2, 3, 4, 5	
$[X]_{cd}(t) = [X]_c(t-\theta_d)$	(3.4)
where X is W, AD, L(q) with q = 1, 2, 3, 4, 5	
$\frac{dm_{cc}}{dt} = F_{gtot}L_f M_{L_f}$	(3.5)
$m_{cc_d}(t) = m_{cc}(t-\theta_d)$	(3.6)

The second term on the right-hand side of (3.1) accounts for water that leaves the condenser, assuming that the condenser liquid is well mixed. Note that M_{Lf} is the average molar mass of the liquid in the condenser, which is computed from the liquid composition. The unknown mass hold-up in the condenser, m_c, is an additional model parameter that requires estimation. ODEs (3.2) and (3.3) are similar in structure to ODE (3.1) and do not contain any additional parameters. ODE (3.5) is a mass balance that predicts m_{cc}, the total mass of liquid that would have accumulated in the condensate collector if there were no time delay in the system. Equations

(3.4) and (3.6) account for the time delay θ_d in the concentrations of the condensate entering the condensate collector and in the mass of liquid in the condensate collector. The subscript d indicates that these predictions account for the delay. The equations in Table 3 were used to augment the model of Cui et al., increasing the total number of unknown parameters from 18 to 20 due to the additional parameters m_c and θ_d. Time delay arises from two sections of piping, but Laplace transforms can be used to confirm that only a single total-delay parameter θ_d is warranted in the model.

The following objective function was used for parameter estimation and for computation of the MSE-based criterion r_{cc} using the algorithm in Table 2:

$$
\begin{aligned}
J = {} & \frac{1}{s_{L(1)}^2}\sum\left([L(1)]_m - [L(1)]\right)^2 + \sum_{q=2}^{7}\frac{1}{s_{L(q)}^2}\sum\left([L(q)]_m - [L(q)]\right)^2 \\
& + \frac{1}{s_W^2}\sum\left([W]_m - [W]\right)^2 + \frac{1}{s_{AD}^2}\sum\left([AD]_m - [AD]\right)^2 \\
& + \frac{1}{s_O^2}\sum\left([O]_m - [O]\right)^2 + \frac{1}{s_U^2}\sum\left([U]_m - [U]\right)^2 \\
& + \sum_{q=1}^{5}\frac{1}{s_{L(q)_c}^2}\sum\left([L(q)]_{cdm} - [L(q)]_{cd}\right)^2 \\
& + \frac{1}{s_{W_c}^2}\sum\left([W]_{cdm} - [W]_{cd}\right)^2 + \frac{1}{s_{AD_c}^2}\sum\left([AD]_{cdm} - [AD]_{cd}\right)^2 \\
& + \frac{1}{s_{m_{cc}}^2}\sum\left(m_{ccd_m} - m_{ccd}\right)^2 \qquad (4)
\end{aligned}
$$

The first six terms on the right-hand side involve measured concentrations (denoted by the subscript m) of species in the reactor including monomer $[L(1)]_m$, linear oligomers $[L(q)]_m$, q = 2 to 7, water $[W]_m$, propanal $[AD]_m$, hydroxyl ends $[O]_m$, and unsaturated ends $[U]_m$. The next three terms involve measurements of species concentrations leaving the condenser, which were influenced by time delay. The final term involves measurements of the mass of liquid in the condensate collector, which are also influenced by the time delay. Altogether, 727 data values were available to fit the 20 model parameters. These data arose from four dynamic experiments conducted using four different catalyst levels (Cui et al., 2015). Note that concentration measurements were available for oligomeric species with lengths up to 7; however, hexamer and heptamer are sufficiently non-volatile that their concentrations in the condenser liquid are negligible. Measurement uncertainty weighting factors s_X that appear in the denominators of the various terms in the objective function were set based on measurement uncertainty information provided by the industrial sponsor who performed the experiments (Cui et al., 2015). These same uncertainties were used as the corresponding s_{yi} values in the ranking algorithm (see Table 1).

All of the sensitivity coefficients required to rank the parameters were obtained using difference approximations wherein each parameter was adjusted one-at-a-time by 5 % of its initial guess. It is important to use reasonably large perturbations in the parameters so that the predicted changes Δg_d in the responses are large compared to numerical errors associated with solving the ODEs. Cui et al. (2015) provide values of the initial guesses and uncertainty scaling factors for the 18 kinetic and mass-transfer parameters that appear in the original delay-free model. Initial guesses for m_c and θ_d were set at 0.15 kg and 0.15 h, respectively, based on our knowledge of the size and typical flow rates in the condenser system. The lower bounds for these additional parameters were set at 0.1 kg and 0.05 h, respectively, and the corresponding upper bounds were set at 0.5 kg and 0.5 h. The corresponding uncertainties s_{mc} and $s_{\theta d}$ required for the parameter ranking algorithm in Table 1 were set at half the distance between the respective upper and lower bounds. No adjustments to the ranking algorithm in Table 1 were required to accommodate the time delay beyond including the corresponding time-delay column in the scaled sensitivity matrix and formulating the model equations so that the delay parameter θ_d appears explicitly in (3.4) and (3.6). No changes to the algorithm in Table 2 were required to accommodate the unknown time-delay parameter.

4. RESULTS

The complete set of model parameters (including m_c and θ_d) was ranked from most estimable to least estimable, with m_c appearing 10th and θ_d appearing 11th. Use of the selection algorithm in Table 2 indicated that 18 parameters should be estimated using the available data. Note that one of the parameters (the equilibrium constant for polycondensation) that Cui et al. could not estimate using the delay-free model became estimable (with its rank improving to 13th) using the extended model that accounts for delay. Using the resulting estimates for the 18 parameters resulted in an objective function value of $J = 3.6 \times 10^5$ compared with 7.6×10^6 obtained from (4) using the parameter estimates and model of Cui et al., which did not account for delay and condensate hold-up.

Selected model predictions for several of the state variables obtained using the proposed methodology are shown in Fig. 2 and Fig. 3. Fig. 2 compares predictions of the model with time delay (solid curve) and Cui's predictions without time delay (dashed curve) with experimental data for m_{cc}, the mass of liquid accumulated in the condensate collector during one of the runs (see Fig. 1). As expected, the model (and associated parameter estimates) that accounts for time delay and condensate hold-up provides a much better fit to the data.

Fig. 3 shows comparisons between the model predictions with experimental data for the concentration of dimer and tetramer in the polymerization reactor. These data were obtained during the same experimental run as the data in Fig. 2. As shown by the dashed curves, one of the problems with the previous delay-free model and parameter estimates of Cui et al. (2015) is that they predict maxima in the concentrations of these (and the other oligomers) that are earlier in time than the corresponding maxima in the measured data. The extended model (and parameter estimates obtained using the proposed methodology) predicts locations for maxima that are close to those for the experimental maxima.

We note, however, that there is considerable mismatch between the predicted and measured oligomer concentrations

at long reaction times, suggesting that estimates for the equilibrium constant for polycondensation and/or the mass-transfer coefficient for removal of water may be too small. As a result, we suspect that the optimizer (lsqnonlin in MATLAB) may have converged to a local optimum. Users of the proposed methodology should be aware of the possibility of finding local minima, especially when using models with numerous parameters that have a nonlinear influence on the model predictions (McLean et al., 2012b). To deal with this issue, we recommend re-starting the parameter ranking, selection and estimation procedure at a variety of different initial guesses from within the set of possible parameter values. These initial guesses can either be selected randomly or based on the engineering judgment of the modeler (Woloszyn and McAuley, 2011). The proposed extension that readily accounts for time-delay as one of the parameters will enable our ongoing study of the parameter space in order to find a better minimum for J and a corresponding better fit to the polymerization data.

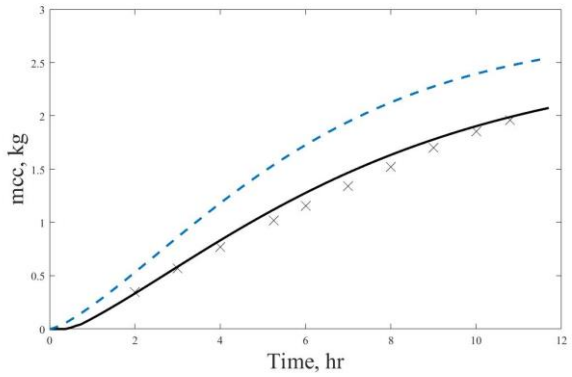

Fig. 2. Model prediction for mass accumulated in the condensate collector (× measured data, -- prediction without time delay, − prediction with time delay)

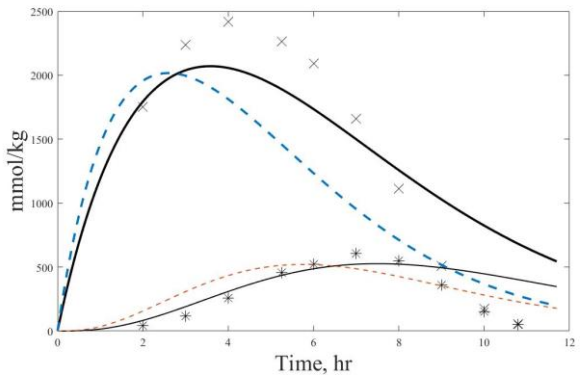

Fig. 3. Model prediction for concentration of dimer and tetramer in the reactor (dimer: × measured data, -- prediction without time delay, ─ prediction with time delay; tetramer: * measured data, - - prediction without time delay, − prediction with time delay)

4. CONCLUSIONS

A proposed extension is developed for a methodology that ranks parameters according to their estimability and selects an appropriate subset for estimation. This methodology uses difference approximations for sensitivity coefficients making it straightforward to consider unknown time delay as a parameter that may require estimation. The proposed methodology relies on earlier algorithms for ranking model parameters (Yao et al., 2003; Thompson et al., 2009) and for finding the optimal number of parameters for estimation (Wu et al., 2011; McLean and McAuley, 2012a). However, a similar approach could also be used for handling time delay in other sensitivity-based selection techniques. (Weijers and Vanrolleghem, 1997; Sun and Hahn, 2006; Chu and Hahn, 2007; Chu et al., 2009; Eghtesadi and McAuley, 2016).

A polymerization batch reactor model is used to illustrate the effectiveness of the proposed method. An improved fit to the data is obtained compared with prior model fits obtained by Cui et al. (2015) using a delay-free model. Although, the resulting estimates lead to better predictions on average, it is apparent that a more rigorous estimation procedure should be attempted, starting from a variety of initial parameter guesses to explore whether the optimum with $J = 3.6 \times 10^5$ is only a local optimum. If a better optimum cannot be found, we may need to extend the model to account for formation of cyclic oligomers, which have been ignored in the current reactor model (Cui, 2014). Incorporating additional reactions and species will lead to additional ODEs and model parameters, making it even more important to have available an easy-to-use parameter ranking and selection tool that accounts for time delay and will prevent over-fitting while determining an appropriate subset of parameters to estimate.

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