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There are three ways by which the value of unknown parameters in a process model may be determined as;

1. Extracting needed parameters from the published literature.
2. Conveying out independent experiments to determine fundamental model parameters; for example lab experiments for determining kinetic rate constants, to be used in a model for a full scale industrial reactor.
3. Performing experiments on the particular physical systems of interest and determine the unknown parameter values that produce model predictions that are closest fit to the experimentally observed data.

When the required parameters are unavailable in the literature, the only other alternative is to estimate them from experimental data.

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For parameter estimation purposes, the theoretical model for any process can be represented in the following form;

$$\eta = f(Z, \quad) \hspace{6cm} 5.1$$

where;

$\eta=$ an n-dimensional vector of actual process output that can be measured in an experiment.

= an m-dimensional vector of independent variables that can be specified arbitrarily for each experiment, or variables that, for each experimental observation are known precisely.

= is a P-dimensional vector of the unknown parameter.

f= some functional relationship between these above variables, it may be an explicit functional relationship , or an analytical solution to a differential equation model, it may also be an implicit function as in the differential equation itself but the form f takes is unknown.

Example: Explicit functional form for the Model of Isothermal Batch Reactor

A batch reactor is one in which the isothermal 1st order conversion of reactant A to product is taking place and is modeled by;

$$\frac{dC_A}{dt} = -kC_A \qquad\qquad 5.2$$

This is linear first order O.D.E whose solution is given as;

$$C_A = C_{A0}e^{-kt} \qquad\qquad 5.3$$

Observe that eq. (3) is in the form of eq. (1) with

$$\eta = C_A; \; Z = [C_{A0}, t]; \Theta = k$$

Linear or non linear parameter estimation

The parameter estimation is said to be linear or non linear with regards to the vector of parameters and not with regards to the state variables. IF in eq 1 function t is linear with respect to the vector then the model is said to be linear in the parameters estimation when the parameters enter the model in a nonlinear fashion we have a nonlinear parameter estimation.

to check the parameter estimation problem for linearity obtain $\frac{\partial f}{\partial \theta}$, if the result is independent of then the problem is linear in otherwise it is a nonlinear in that parameter.

Elements of parameter estimation

each single experiment involves measuring all the n output variables $_1$ $_2$…. $_n$ for a specified set of values for the independent variables z1 , z2 …. zn. In order to determine the p parameters $\theta 1, \theta 2, ….. \theta p$

independently. It is necessary to perform at least p such experiments. The greater the number of experiments performed better our estimates will be.

the result of each individual experiment is a set of vector and z that may be related to the process model in particular for the kth experiment we have

$$(k) = f(z(k), \theta); \; k = 1,2….N \qquad\qquad 5.4$$

N= no of separate experiments have been performed.

We now note that the experimental measurements of (k) will not be exactly equal to its true value because of measurement error. Hence we differentiate the actual process output (k) from its experimentally observed measurement denoted by y(k)

$$y(k) = f(z(k), \theta) + E(k); \; k = 1,2….N \qquad\qquad 5.5$$

where E(k) is the vector of errors between the model prediction and the actual data.

Parameter estimation is now involved to find a specific set of parameters value θ such that osme scalar function S of the error vector known as objective function and usually represented as $S(\theta)$ since it depends on the θ parameter value is minimized over the entire range of possible value of θ. The smallest value of $S(\theta)$ is given by $S(\bar{\theta})$

Error criterion

Several criteria are used to obtain optimal estimates of unknown model parameters but the most widely used is the least square criterion. In this case the sum of squares of the errors is the function to be minimized

$$S(\theta) = \sum_{k=1}^{N}[E(k)]^T[E(k)] \qquad \qquad 5.6$$

$$S(\theta) = \sum_{k=1}^{N}[y(k) - f(z(k), \ )]^T[y(k) - f(z(k), \ )] \qquad \qquad 5.7$$

where the summation is over all the data points.

Some times it might be necessary to assign more weight to more precise measurements and less less weight to the others. This is accomplished by introducing a weighting matrix as follows:

$$S(\theta) = \sum_{k=1}^{N}[y(k) - f(z(k), \ )]^T w(k)[y(k) - f(z(k), \ )] \qquad \qquad 5.8$$

where w(k) is the n*n weighting matrix where elements reflect the relative precision of various measurements (weighting least squares)

Parameter estimation in Differential equation models with analytical solution:

When the process model is such that it possess an analytical solution the parameter estimation problem is made such that much easier since an explicit expression of the form gicen in eq 1 is obtained directly from the analytical solution

case I $f(z, \theta)$ is linear in θ

case II $f(z, \theta)$ is non linear in θ

Linear Estimation:

When the analytical solution of a process model is obtained in the form

$$= f(z, \theta) \qquad \qquad 5.9$$

then from Eq(5.9) we see that the experimentally obtained measurements of process output (which we have referred as y(k) obtained for various values of the vector of independent variables, z(k) are related to the process modeled according to

$$
\begin{bmatrix} y(1) \\ y(2) \\ \vdots \\ \cdot \\ y(N) \end{bmatrix} = \begin{bmatrix} f(z(1),\theta) \\ f(z(2),\theta) \\ \vdots \\ \cdot \\ f(z(N),\theta) \end{bmatrix} + \begin{bmatrix} E(1) \\ E(2) \\ \vdots \\ \cdot \\ E(N) \end{bmatrix}
$$
                                                                                                        5.10

if f(z, θ) is linear in the θ then it can be shown that eq(6) becomes

$$ Y = X\,\theta + E $$ 5.11

where X is the complete matrix of independent variables compiled for each data set, Y is the entire collection of the experimentally obtained data E is the collection of errors

The linear parameter estimation is now to find the vector $\hat{\theta}$ for which the squard direction of data set Y from the model X θ is minimized

$$ \hat{\theta} = (X^T X)^{-1} X^T Y $$ 5.12

Example:

The theoretical model for a storage tank

$$ \frac{dh}{dt} = K^* \, (F_i - f) $$

Fi = inlet stream flow rate

f = outlet stream flow rate

metered outlet flow rate

the only process parameters is K* is to be estimated from experimental data

show that for the situation in which a unti step increase is made in the inlet flow rate Fi

$\frac{dh}{dt} = K^*$

$(F_i - f) = 1$

h = K* t +c

$h_o = c$

$h = h_o + K*t$

$_1 = h - h_o$

$z_1 = t$

$_1 = K*$

$_1 = z_1 \quad _1$

If the level measurement at times t_1 t_2 …. tn are respectively h_1 h_2 ….. h_N

$y_1 = h_1 - h_o = K*t_1 + E_1$

………………………………….

………………………………..

$y_N = h_N - h_o = K*t_N + E_N$

$$\begin{bmatrix} y(1) \\ y(2) \\ \vdots \\ \cdot \\ y(N) \end{bmatrix} = \begin{bmatrix} t(1) \\ t(2) \\ \vdots \\ \cdot \\ t(N) \end{bmatrix} K* + \begin{bmatrix} E(1) \\ E(2) \\ \vdots \\ \cdot \\ E(N) \end{bmatrix}$$

$Y = X\,\theta + E$

$$X = \begin{bmatrix} t(1) \\ t(2) \\ \vdots \\ \cdot \\ t(N) \end{bmatrix}$$

$$Y = \begin{bmatrix} y(1) \\ y(2) \\ \vdots \\ \cdot \\ y(N) \end{bmatrix}$$

If we apply Eq(5.12) using these specific vectors we obtain that K* the least square estimates of K*

$$X = \begin{bmatrix} t(1) \\ t(2) \\ \vdots \\ \cdot \\ t(N) \end{bmatrix} \qquad X^T = \begin{bmatrix} t1 & t2 & \cdot & \cdot & t_N \end{bmatrix}$$

$$X^T X = \begin{bmatrix} t1 & t2 & \cdot & \cdot & t_N \end{bmatrix} \begin{bmatrix} t(1) \\ t(2) \\ \vdots \\ \cdot \\ t(N) \end{bmatrix}$$

$$= \sum_{k=1}^{N} t_k^2$$

$$X^T Y = \begin{bmatrix} t1 & t2 & \cdot & \cdot & t_N \end{bmatrix} \begin{bmatrix} y(1) \\ y(2) \\ \vdots \\ \cdot \\ y(N) \end{bmatrix}$$

$$= \sum_{k=1}^{N} t_k y_k$$

$$\widehat{K^*} = \frac{\sum_{k=1}^{N} t_k y_k}{\sum_{k=1}^{N} t_k^2}$$

Non linear Estimation:

The more common situation with process models for which analytical solutions exist is for the functional form of f(z, θ) to be nonlinear in   e.g. for any first order system

$$\tau \frac{dy}{dx} + y = Ku(t) \qquad\qquad 5.13$$

The general solution to this model for a unit step input in u(t) is

$$y(t) = K\,(1\text{-}e^{-t/\tau}) \qquad\qquad 5.14$$

which is linear in K but nonlinear in τ non linear estimation problems are handled in general by numerical techniques

Linearize to model by taking its log in both sides

$$1 - \frac{y(t)}{K} = e^{-t/\tau}$$

$$ln\left\{1 - \frac{y(t)}{K}\right\} = -t/\tau \qquad\qquad 5.15$$