7.3.1 Soft Sensors

One of the common problems shared by many industrial processes is the inability to measure key process variables noninvasively and in real time, especially the compositions of process streams and product properties. The development of improved sensors, based on new techniques of analytical chemistry and modern electronic devices using fiber optics and semiconductors, has been an active area (cf. Appendix A). As an alternative, the use of easily measured secondary variables to infer values of unmeasured process variables is now receiving great interest; the term *virtual soft sensors* or *sensors* (Martin, 1997) is often used to denote this approach. *Chemometrics* is a term related to soft sensors that describes how data from process analyzers (e.g., spectra) can be analyzed and modeled for use in process monitoring and control (Brown, 1998).

Soft sensors have become an attractive alternative to the high cost of accurate on-line measurements for applications where empirical models can accurately infer (that is, predict) unmeasured variables. For example, the environmental regulatory agency in Texas now permits NN models to be used for monitoring emissions from various process units such as power boilers. The NN models use measurements of selected input and output variables to predict pollutants at the parts per billion level (Martin, 1997). In materials manufacturing, the real-time detection of cracks, inclusions, porosity, dislocations, or defects in metallurgical or electronic materials would be highly desirable during processing, rather than after processing is completed and defective products are shipped. Use of virtual sensor models to predict quality control measures, such as the formation and location of defects, can greatly reduce the stringent requirements imposed on hardware-based sensors.

7.4 DEVELOPMENT OF DISCRETE-TIME DYNAMIC MODELS

A digital computer by its very nature deals internally with discrete-time data or numerical values of functions at equally spaced intervals determined by the sampling period. Thus, discrete-time models such as *difference equations* are widely used in computer control applications. One way a continuous-time dynamic model can be converted to discrete-time form is by employing a finite difference approximation (Hanna and Sandall, 1995). Consider a nonlinear differential equation,

$$\frac{dy(t)}{dt} = f(y, u) \tag{7-26}$$

where y is the output variable and u is the input variable. This equation can be numerically integrated (though with some error) by introducing a finite difference approximation for the derivative. For example, the first-order, backward difference approximation to the derivative at $t = k\Delta t$ is

$$\frac{dy}{dt} \cong \frac{y(k) - y(k-1)}{\Delta t} \tag{7-27}$$

where Δt is the integration interval specified by the user and $y(k)$ denotes the value of $y(t)$ at $t = k\Delta t$. Substituting Eq. 7-26 into (7-27) and evaluating $f(y, u)$ at the previous values of y and u (i.e., $y(k-1)$ and $u(k-1)$) gives:

$$\frac{y(k) - y(k-1)}{\Delta t} \cong f(y(k-1)), u(k-1)) \tag{7-28}$$

$$y(k) = y(k-1) + \Delta t\, f(y(k-1), u(k-1)) \tag{7-29}$$

Equation 7-29 is a first-order difference equation that can be used to predict $y(k)$ based on information at the previous time step $(k-1)$. This type of expression is called a *recurrence relation*. It can be used to numerically integrate Eq. 7-26 by successively calculating $y(k)$ for $k = 1, 2, 3, \ldots$ starting from a known initial condition $y(0)$ and $u(k)$. In general, the resulting numerical solution becomes more accurate and approaches the correct solution $y(t)$ as Δt decreases. However, for extremely small values of Δt, computer roundoff can be a significant source of error (Hanna and Sandall, 1995).

EXAMPLE 7.4

For the first-order differential equation,

$$\tau \frac{dy(t)}{dt} + y(t) = Ku(t) \tag{7-30}$$

derive a recursive relation for $y(k)$ using a first-order backwards difference for dy/dt.

SOLUTION

The corresponding difference equation after approximating the first derivative is

$$\frac{\tau(y(k) - y(k-1))}{\Delta t} + y(k-1) = Ku(k-1) \tag{7-31}$$

Rearranging gives

$$y(k) = \left(1 - \frac{\Delta t}{\tau}\right)y(k-1) + \frac{K\,\Delta t}{\tau}u(k-1) \tag{7-32}$$

The new value $y(k)$ is a weighted sum of the previous value $y(k-1)$ and the previous input $u(k-1)$. Equation 7-32 can also be derived directly from (7-29). ■

As shown in numerical analysis textbooks, the accuracy of Eq. 7-32 is influenced by the integration interval. However, discrete-time models involving no approximation errors can be derived for any linear differential equation under the assumption of a piecewise constant input signal, that is, the input variable u is held constant over Δt. Next, we develop discrete-time modeling methods that introduce no integration error for piecewise constant inputs, regardless of the size of Δt. Such models are important in analyzing computer-controlled processes where the process inputs are piecewise constant.

7.4.1 Exact Discrete-Time Models

For a process described by a linear differential equation, the corresponding discrete-time model can be derived from the analytical solution for a piecewise constant input. This analytical approach eliminates the discretization error inherent in finite-difference approximations. Consider a first-order model in Eq. 7-30 with previous output $y[(k-1)\Delta t]$ and a constant input $u(t) = u[(k-1)\Delta t]$ over the time interval $(k-1)\,\Delta t \leq t < k\Delta t$. The analytical solution to Eq. 7-30 at $t = k\Delta t$ is

$$y(k\Delta t) = (1 - e^{-\Delta t/\tau})Ku[(k-1)\Delta t] + e^{-\Delta t/\tau}y[(k-1)\Delta t] \tag{7-33}$$

Equation 7-33 can be written more compactly as

$$y(k) = e^{-\Delta t/\tau}y(k-1) + K(1 - e^{-\Delta t/\tau})u(k-1) \tag{7-34}$$

Equation 7-34 is the exact solution to Eq. 7-30 at the sampling instants provided that $u(t)$ is constant over each sampling interval of length Δt. Note that the continuous output $y(t)$ is not necessarily constant between sampling instants, but (7-33) and (7-34) provide an exact solution for $y(t)$ at the sampling instants, $k = 1, 2, 3, \ldots$.

In general, when a linear differential equation of order p is converted to discrete time, a linear difference equation of order p results. For example, consider the second-order model:

$$G(s) = \frac{Y(s)}{U(s)} = \frac{K(\tau_a s + 1)}{(\tau_1 s + 1)(\tau_2 s + 1)} \tag{7-35}$$

The analytical solution for a constant input provides the corresponding difference equation, which is also referred to as an autogressive model with external (or exogenous) input, or *ARX model* (Ljung, 1999):

$$y(k) = a_1y(k-1) + a_2y(k-2) + b_1u(k-1) + b_2u(k-2) \tag{7-36}$$

where

$$a_1 = e^{-\Delta t/\tau_1} + e^{-\Delta t/\tau_2} \tag{7-37}$$

$$a_2 = -e^{-\Delta t/\tau_1}e^{-\Delta t/\tau_2} \tag{7-38}$$

$$b_1 = K\left(1 + \frac{\tau_a - \tau_1}{\tau_1 - \tau_2}e^{-\Delta t/\tau_1} + \frac{\tau_2 - \tau_a}{\tau_1 - \tau_2}e^{-\Delta t/\tau_2}\right) \tag{7-39}$$

$$b_2 = K\left(e^{-\Delta t(1/\tau_1 + 1/\tau_2)} + \frac{\tau_a - \tau_1}{\tau_1 - \tau_2}e^{-\Delta t/\tau_2} + \frac{\tau_2 - \tau_a}{\tau_1 - \tau_2}e^{-\Delta t/\tau_1}\right) \tag{7-40}$$

In Eq. 7-36 the new value of y depends on the values of y and u at the two previous sampling instants; hence, it is a second-order difference equation. If $\tau_2 = \tau_a = 0$ in Eqs. 7-36 through 7-40, the first-order difference equation in (7-33) results.

The steady-state gain of the second-order difference equation model can be found by considering steady-state conditions. Let $\bar{u}$ and $\bar{y}$ denote the new steady-state values after a step change in u. Substituting these values into Eq. 7-36 gives

$$\bar{y} = a_1\bar{y} + a_2\bar{y} + b_1\bar{u} + b_2\bar{u} \tag{7-41}$$

Because y and u are deviation variables, the steady-state gain is simply $\bar{y}/\bar{u}$, the steady-state change in y divided by the steady-state change in u. Rearranging Eq. 7-41 gives

$$\text{Gain} = \frac{\bar{y}}{\bar{u}} = \frac{b_1 + b_2}{1 - a_1 - a_2} \tag{7-42}$$

Substitution of Eqs. 7-37 through 7-40 into (7-42) gives K, the steady-state gain for the transfer function model in Eq. 7-35.

Higher-order linear differential equations can be converted to a discrete-time, difference equation model using a state space analysis (Åström and Wittenmark, 1997).

7.5 IDENTIFYING DISCRETE-TIME MODELS FROM EXPERIMENTAL DATA

If a linear discrete-time model is desired, one approach is to fit a continuous-time model to experimental data (cf. Section 7.2) and then to convert it to discrete-time form using the above approach. A more attractive approach is to estimate parameters in a discrete-time model directly from input-output data based on linear regression. This approach is an example of *system identification* (Ljung, 1999). As a specific example, consider the second-order difference equation in (7-36). It can be used to predict $y(k)$ from data available at time $(k-1)\Delta t$ and $(k-2)\Delta t$. In developing a discrete-time model, model parameters a_1, a_2, b_1, and b_2 are considered to be unknown. They are estimated by applying linear regression to minimize the error criterion in Eq. 7-8 after defining

$$\beta^T = [a_1\ a_2\ b_1\ b_2], \quad X_1 = y(k-1), \quad X_2 = y(k-2), \quad X_3 = u(k-1), \quad \text{and} \quad X_4 = u(k-2)$$

EXAMPLE 7.5

Consider the step response data $y(k)$ in Table 7.2, which were obtained from Example 7.3 and Fig. 7.8 for $\Delta t = 1$. Initially, the system is at rest. At $t = 0$ a unit step change in u occurs, but the first output change is not observed until the next sampling instant. Estimate the model parameters in the second-order difference equation (7-36) from the input-output data. Compare this model with the models obtained in Example 7.3 using nonlinear regression.