Generalized Likelihood Ratios for Gross Error Identification in Dynamic Processes

Gross error identification in dynamic processes is important in ensuring proper process control. This paper describes the application of a generalized likelihood ratio (GLR) method for identifying gross errors caused by biases in measuring instruments and controllers, process leaks, and failure of controllers. As shown in the application to steady state processes (Narasimhan and Mah, 1987), this method provides a general framework for identifying different types of gross errors whose effect on the process can be modeled. An important feature of the work is the treatment of closed-loop dynamic processes. The formulation of the hypotheses of the GLR method proposed by Willsky and Jones (1974) is extended for this purpose. For estimating the time of occurrence of the gross error, a simple chi-square test on the innovations (measurement residuals) is used, which is computationally more efficient than the method used by Willsky and Jones. Through simulation studies of a level control process the appropriate selection of parameters of the GLR method is investigated.

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Introduction

Gross errors caused by biases in measuring instruments and controllers, material and energy losses due to leaks, and failure of measuring instruments and controllers adversely affect the performance of a process. Timely identification of these gross errors is useful in obtaining reliable estimates of process variables leading to improved process control and also improves the overall maintenance of a plant.

Considerable effort has been expended on developing methods for gross error identification in steady state chemical processes (Tamhane and Mah, 1985; Mah, 1987). But in reality a process is probably never truly in a steady state. Even a so-called steady state process is constantly undergoing variations about a nominal steady state. A dynamic process model represents a better approximation of an actual process. A second important reason for considering dynamic processes arises from the need to adequately describe the effect of controllers on a process and to identify gross errors associated with them.

In chemical engineering, relatively little effort has gone into the development of gross error identification methods for dynamic processes. Even the methods proposed so far (Bellingham and Lees, 1977; Newman, 1982; Watanabe and Himmelblau, 1982) are specifically intended for identifying measurement biases, and do not offer a general framework for identifying different types of gross errors.

In a previous paper (Narasimhan and Mah, 1987), we described a generalized likelihood ratio (GLR) method that provides a general framework for identifying any type of gross error that can be modeled. In this paper, we describe the methodology for gross error identification in dynamic processes. We illustrate the application of this method for identifying gross errors caused by biases in measuring instruments and controllers, process leaks, and failure of controllers. We restrict our considerations only to linear, dynamic processes that are corrupted by normally distributed process noise and measurement noise. Moreover, we consider only dynamic processes operated around a nominal steady state. The methodology we develop is not applicable to process start-up nor to processes undergoing a transition from one steady state to another.

The GLR method was first proposed and used by Willsky and Jones (1974) for identifying abrupt steps or jumps in the state

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variables and measurements. We have made several important extensions to this method. We first extend the method to treat closed-loop dynamic systems with the control law included. Hitherto, the system inputs from controllers (hereafter termed control inputs) have been taken as constants (Willsky and Jones, 1974) or assumed to be unaffected by the presence of a gross error (Watanabe and Himmelblau, 1982). But it is more realistic to assume that the control inputs are either functions of state estimates or functions of measurements, and are therefore affected by the presence of a gross error. In our work, we treat multivariable control laws that are linear functions of estimates. Secondly, we extend the formulation of the hypotheses for gross error identification, which enables us to identify failure of controllers. Lastly, we propose an efficient method for estimating the time of occurrence of the gross error by making use of a statistical test, referred to as the time of occurrence detection (TOD) test.

A level control process is chosen as an example, and simulation studies are performed to illustrate the effectiveness of the GLR method and also to guide the selection of important parameters of the method. Our results show that by choosing a low value for the level of significance of the TOD test, we can obtain better performance in identifying gross errors.

Process and Measurement Model

The dynamic behavior of a process is described by a set of differential equations that represent the mass and energy balances of the process. From these differential equations a linear discrete process model is obtained, which can be written as

$$\underline{x}_{k+1} = \underline{A}_k \underline{x}_k + \underline{B}_k \underline{u}_k + \underline{\Gamma}_k \underline{w}_k \quad (1)$$

where $\underline{x}_k$:$s \times 1$ is a vector of state variables at time instant k; $\underline{A}_k$:$s \times s$ is the state transition matrix; $\underline{u}_k$:$m \times 1$ is a vector of control inputs and $\underline{B}_k$:$s \times m$ is the corresponding input matrix; $\underline{w}_k$:$p \times 1$ is assumed to be a normally distributed process noise vector with mean $\underline{0}$ and known covariance matrix $\underline{R}_k$; and $\underline{\Gamma}_k$:$s \times p$ is the corresponding noise matrix. The subscript k for all variables denotes time instant k. In addition we have a linear control law

$$\underline{u}_k = \underline{C}_k \hat{\underline{x}}_{k|k} \quad (2)$$

where $\hat{\underline{x}}_{k|k}$ are the estimates of the state variables, given measurements up to time k. These estimates are obtained by using the Kalman filter equations (Kalman, 1960), which are given in Supplementary Material 1.

The measurements $\underline{z}_k$ are given by

$$\underline{z}_k = \underline{H}_k \underline{x}_k + \underline{v}_k \quad (3)$$

where $\underline{v}_k$:$n \times 1$ is assumed to be a vector of normally distributed random measurement noise with mean $\underline{0}$ and known covariance matrix $\underline{Q}_k$. It is also assumed that the process noise and the measurement noise are white noises; that is, the expected values of $\underline{w}_j \underline{w}'_k$ and $\underline{v}_j \underline{v}'_k$ are equal to zero for $j \neq k$. It is further assumed that the process noise and measurement noise are mutually independent; that is, the expected value of $\underline{w}_j \underline{v}'_j$ is equal to zero for all j and k. If the process is operated around a nominal steady state, then the system matrices, $\underline{A}_k$, $\underline{B}_k$, Γ_k, $\underline{H}_k$, $\underline{R}_k$, and $\underline{Q}_k$ may be treated as constants. If the operating steady state changes, then these system matrices need to be recalculated.

Review of Past Work

In systems engineering the term "failures" has been used instead of gross errors. As pointed out earlier, the GLR method was developed by Willsky and Jones (1974) for indentifying failures caused by abrupt steps or jumps in the state variables. Later, in a review of different methods for failure detection, Willsky (1976) also developed the models for describing the effect of a controller failure and measuring instrument failure. Tylee (1983) applied the GLR method for identifying measurement biases in nuclear power plant instrumentation. Several other methods that are available for failure detection and identification have been reviewed by Willsky (1976), and by Isermann (1984). The methods that were applied to nuclear power plants for identifying failures in measuring instruments have been reviewed by Upadhyaya (1985). Most of the methods are specifically developed for identifying biases in measurements. Among the different methods, only the GLR method has the capability of identifying different types of failures. Hence we have chosen to use this approach for gross error identification.

In chemical engineering, a method for the detection and estimation of biases in measurements was developed by Bellingham and Lees (1977). Newman (1982) suggested a procedure for processing the measurements, one by one in a serial manner, for identifying biases in measurements. Park and Himmelblau (1983) proposed a method for identifying specific faults, such as fouling of heat exchange and blockage of pipes, by estimating the parameters (heat transfer coefficient and flow rate) associated with these faults and comparing the estimates with nominal values. Watanabe and Himmelblau (1982) proposed a method for identifying biases and failures in measuring instruments in certain classes of nonlinear processes. The method, however, makes a restrictive assumption that the control inputs at all times are not affected by these gross errors. Himmelblau (1986) has also reviewed techniques for fault detection and diagnosis. However, there is a paucity of methods for identifying different types of gross errors in chemical processes. Even the methods that have been developed in the field of systems engineering have not been adapted to chemical processes. Thus a natural direction to pursue is to examine whether existing techniques in systems engineering can be adapted for gross error identification in chemical processes.

Gross Error Models

A gross error model describes the effect of a gross error on the process. We describe the models for four different types of gross errors assuming that each gross error occurs as a step change. We also assume that the magnitude of the gross error, b, and the time at which it occurs, t, are unknown but fixed nonrandom quantities.

Process leak model

A leak of magnitude b in process unit j that occurs at time t can be modeled as a step change in the state equations

$$\underline{x}_{k+1} = \underline{A}_k \underline{x}_k + \underline{B}_k \underline{u}_k + b \underline{m}_j \sigma_{k-t} + \underline{\Gamma}_k \underline{w}_k \quad (4)$$

where

$$\sigma_{k-t} = \begin{cases} 0 & \text{if } k < t \\ 1 & \text{if } k \geq t \end{cases} \tag{5}$$

Since a leak in a process unit affects the material and energy balances, and the state equations are also derived from material and energy balances, we can intuitively confirm that the above model is reasonable. The vector $\underline{m}_j$ that corresponds to the leak in unit j, is obtained as follows. The differential equations for material and energy balances are augmented by a term of the form $b\underline{m}_j^*$. The vector $\underline{m}_j^*$ has nonzero elements corresponding to the differential equations that are associated with unit j. For mass balance equations, the corresponding nonzero element is unity, and for energy (resp., component) balance equations, the corresponding nonzero entries are chosen to be equal to the nominal enthalpy (resp., concentration) of the fluid contained in the process unit. Alternatively, the method that we proposed for constructing the leak model in the steady state case (Narasimhan and Mah, 1987) may be used. When the differential equations are linearized and discretized, the vector for the process leak is transformed to give the vector $b\underline{m}_j$. The derivation of a leak vector for a level control process is described in appendix A and Supplementary Material 2.

For certain units, such as a distillation column, enthalpy and concentration vary throughout the length of the column. In this case, more than one leak vector may be necessary for a process unit. However, as stated in the steady state case, good engineering judgment should be exercised and as few leak models should be introduced as necessary to describe the effect of leaks suspected of occurring in the unit. Past experience may indicate where such leaks are likely to occur.

Measurement bias model

If a bias of magnitude b occurs at time t in measurement i, then the measurement model is given by

$$\underline{z}_k = \underline{H}_k \underline{x}_k + b\underline{e}_i \sigma_{k-t} + \underline{v}_k \tag{6}$$

Controller bias model

A bias of magnitude b in controller i occurring at time t can be modeled by the control law

$$\underline{u}_k = \underline{C}_k \hat{\underline{x}}_{k|k} + b\underline{e}_i \sigma_{k-t} \tag{7}$$

Controller failure model

The control law in the presence of a failure of controller i can be modeled as

$$\underline{u}_k = \underline{C}_k \hat{\underline{x}}_{k|k} + (b - \underline{e}_i' \underline{C}_k \hat{\underline{x}}_{k|k}) \underline{e}_i \sigma_{k-t} \tag{8}$$

The above model implies that the control input i is a constant of unknown magnitude b, but the other control inputs are obtained through the control law.

Detecting and Identifying Gross Errors

In this paper, we describe the method for detecting and identifying at most one gross error each time the GLR method is applied. The extension of this method for identifying multiple gross errors is described in Narasimhan (1987). For this purpose we make use of "innovations" or measurement residuals, which are defined as

$$\underline{a}_k = \underline{z}_k - \underline{H}_k \hat{\underline{x}}_{k|k-1} \tag{9}$$

where $\hat{\underline{x}}_{k|k-1}$ are the predicted state estimates at time k given all measurements up to and including time $k - 1$. The estimates are calculated using Eq. SM1-6 of Supplemetary Material 1. (All equation numbers designated SM1- or SM2-refer to equations in the corresponding supplementary material available from NAPS.)

Effect of a gross error on the innovations

It is first necessary to compute the effect of a gross error on the innovations at any time. It should be noted that the values of state variables at any time depend also on the variable values at previous times. Therefore, the net effect of the gross error on the state variables and the innovations change from one time to the next. We can recursively compute this effect by making use of the appropriate gross error model and the Kalman filter equations.

Let us assume that a gross error i has occurred at time t. The effect of any gross error on the innovations at any time k greater than t can be expressed in general as

$$\underline{a}_k = \underline{a}_k^1 + b\underline{G}_{k,t,i} \underline{f}_i + \underline{g}_{k,t,i} \tag{10}$$

where $\underline{a}_k^1$ is the innovation vector that will be obtained if no gross errors are present. The matrix $\underline{G}_{k,t,i}$ and the vector $\underline{g}_{k,t,i}$ are referred to as the signature matrix and signature vector, respectively, and depend on the time k at which the innovations are calculated, the time t at which the gross error occurs, and the gross error i that is present. The vector $\underline{f}_i$ depends on the type of gross error and is given by

$$\underline{f}_i = \begin{cases} \underline{e}_i, & i = 1, \ldots, m \text{ for a controller bias or failure} \\ \underline{e}_i, & i = 1, \ldots, n \text{ for a bias in measurement } i \\ \underline{m}_i, & i = 1, \ldots, q \text{ for a leak in unit } i \end{cases} \tag{11}$$

The recurrence equations for computing the signature matrices and vectors for the different types of gross errors are given in appendix B.

Statistical properties of innovations

In this section we derive the conditional statistical properties of $\underline{a}_k$ given $\underline{Z}_{k-1}$ in the absence and presence of a gross error, where $\underline{Z}_{k-1}$ denotes the set of measurements prior to time k. We use the term "conditional statistical properties" of $\underline{a}_k$ (conditional mean, conditional covariance matrix, etc.) to refer to the statistical properties based on the conditional distribution of $\underline{a}_k$ given the previous measurements $\underline{Z}_{k-1}$.

If no gross errors are present, then the conditional distribution of $\underline{a}_k$ is normal. The mean and covariance matrix of $\underline{a}_k$ are given by Maybeck (1979, p. 229):

$$E[\underline{a}_k | \underline{Z}_{k-1}] = \underline{0} \tag{12}$$

$$\text{cov}\,[\underline{a}_k|\underline{Z}_{k-1}] = \underline{H}_k\underline{P}_{k|k-1}\underline{H}'_k + \underline{Q}_k = \underline{V}_k \quad (13)$$

where $\underline{P}_{k|k-1}$ is the covariance matrix of errors in state estimates obtained from the Kalman filter using Eq. SM1-7. It can also be shown (Maybeck, 1979, p. 228) that

$$\text{cov}\,[(\underline{a}_k|\underline{Z}_{k-1})], (\underline{a}_j|\underline{Z}_{j-1})] = \underline{0} \text{ for } k \neq j \quad (14)$$

In fact, if no gross erros are present, Eqs. 12, 13, and 14 also hold true for unconditioned distribution of $\underline{a}_k$. Equation 14 implies that the innovations at time k are independent of innovations at all times j not equal to k.

When a gross is present, then the innovations are given by Eq. 10. An analysis of each of the three terms on the righthand side of Eq. 10 yields the following observations.

1. We know that $\underline{a}_k^1$ is the innovations that are obtained if no gross errors are present. Therefore, the conditional statistical properties of $\underline{a}_k^1$ are the same as those given by Eqs. 12, 13, and 14.

2. From appendix B, we observe that the signature matrices $\underline{G}_{k,t,i}$ for all gross errors depend only on the system matrices, but not on the measured data. Therefore the signature matrices are constants and not random variables.

3. The signature vectors $g_{k,t,i}$ are equal to $\underline{0}$ for all gross errors that we have considered, except for controller failures. Moreover, it can be observed from Eqs. B18, B14, and B21 that $g_{k,t,i}$ for a controller failure depends only on the state estimates prior to time k, which in turn depends only on all measurements prior to time k. Therefore, given $\underline{Z}_{k-1}$, $g_{k,t,i}$ is a constant.

From the above observations we conclude that in the presence of a gross error, the innovations are normally distributed with conditional statistical properties given by

$$\text{E}\,[\underline{a}_k|\underline{Z}_{k-1}] = b\underline{G}_{k,t,i}\underline{f}_i + g_{k,t,i} \quad (15)$$

$$\text{cov}\,[\underline{a}_k|\underline{Z}_{k-1}] = \text{cov}\,[\underline{a}_k^1|\underline{Z}_{k-1}] = \underline{V}_k \quad (16)$$

Moreover, by using Eqs. 10 and 15, and observation 1 above, we can show that even in the presence of a gross error,

$$\text{cov}\,[(\underline{a}_k|\underline{Z}_{k-1}), (\underline{a}_j|\underline{Z}_{k-1})] = \text{cov}\,[(\underline{a}_k^1|\underline{Z}_{k-1}), (\underline{a}_j^1|\underline{Z}_{j-1})] = \underline{0} \text{ for all } k \neq j \quad (17)$$

Thus even when a gross error is present, the innovations are serially independent, provided conditional statistical properties are used. However, it should be noted that innovations are serially dependent in the presence of a controller failure, when unconditional statistical properties are used. This statistical dependency in the presence of controller failure is caused by the presence of signature vector terms that should be treated as random variables when they are not conditioned on prior measurements.The hypotheses for gross error detection can now be formulated as

$$H_0\colon E[\underline{a}_k|\underline{Z}_{k-1}] = \underline{0}$$
$$H_1\colon E[\underline{a}_k|\underline{Z}_{k-1}] = b\underline{G}_{k,t,i}\underline{f}_i + g_{k,t,i} \quad (18)$$

where f_i is given by Eq. 11.

We detect, identify, and estimate a gross error using N innovations from time t to time $t + N - 1$. The test statistic we use in order to detect a gross error is given by

$$\psi = \sum_{i=t}^{t+N-1} \{(\underline{a}_i)'\underline{V}_i^{-1}(\underline{a}_i)\} \quad (19)$$

Since the innovations under the null hypothesis are serially independent normal variables with mean $\underline{0}$, the above test statistic follows a central chi-square distribution with degrees of freedom equal to Nn. For a given level of significance α_g, we choose as the test criterion, $\chi^2_{Nn,1-\alpha_g}$, the upper $1 - \alpha_g$ quantile of the chi-square distribution with Nn degrees of freedom. We detect a gross error (reject the null hypothesis) if ψ exceeds this criterion. By choosing this criterion, we ensure that the probability of type I error (probability of declaring a gross error when no gross errors are present) is equal to α_g. We refer to this test as the gross error detection (GED) test.

Identification of gross errors

If the GED test detects a gross error, then we have to identify it and estimate its magnitude. For this purpose, we make use of the maximum likelihood ratio (Bickel and Doksum, 1977) and the conditional statistical properties of innovations, as follows.

Let the notation $p\{\underline{X}\}$ represent the joint conditional probability density function of N innovations from time t to time $t + N - 1$. The generalized likelihood ratio may be written as

$$\lambda(\underline{X}) = \sup \frac{p\{\underline{X}\,|\,H_1\}}{p\{\underline{X}\,|\,H_0\}} \quad (20)$$

where the supremum in Eq. 20 is computed over all possible values of the unknown parameters in the hypotheses of Eq. 18. We have shown that the innovations are *serially independent* variables regardless of gross errors, when conditional statistical properties are considered. Therefore, the joint conditional probability density function of the innovations can be obtained easily as a product of the individual conditional density functions of innovations. The conditional expected values and conditional covariance matrices of the innovations in the absence of gross errors are given by Eqs. 12 and 13, respectively, and in the presence of a gross error they are given by Eqs. 15 and 16, respectively. Therefore, the generalized likelihood ratio can written as

$$\lambda(\underline{X}) = \sup_{b,\underline{f}_i} \frac{\exp\left\{-0.5 \sum_{k=t}^{t+N-1} (\underline{\upsilon}_{k,t,i})'\underline{V}_k^{-1}(\underline{\upsilon}_{k,t,i})\right\}}{\exp\left\{-0.5 \sum_{k=t}^{t+N-1} (\underline{a}_k)'\underline{V}_k^{-1}(\underline{a}_k)\right\}} \quad (21)$$

where

$$\underline{\upsilon}_{k,t,i} = \underline{a}_k - b\underline{G}_{k,t,i}\underline{f}_i - g_{k,t,i} \quad (22)$$

In order to simplify the calculation we can compute the quantity

$$T = 2\ln\lambda(\underline{X}) = \sup_{\underline{f}_i} T_i \quad (23)$$

where T_i is given by

$$T_i = \sum_{k=t}^{t+N-1} (\underline{a}_k)'\underline{V}_k^{-1}(\underline{a}_k) - \sup_b \sum_{k=t}^{t+N-1} (\underline{\upsilon}_{k,t,i})'\underline{V}_k^{-1}(\underline{\upsilon}_{k,t,i}) \quad (24)$$

It should be noted that the calculation of T is split into two parts:

Eq. 24 and Eq. 23. The maximum likelihood estimate b_i for every vector $\underline{f}_i$ is obtained by utilizing the necessary condition that the first derivative of the expression on the righthand side of Eq. 24 be equal to zero. Thus,

$$b_i = d_i/C_i \tag{25}$$

where

$$d_i = \underline{f}_i' \sum_{k=t}^{t+N-1} \underline{G}'_{k,t,i} \underline{V}_k^{-1}(\underline{a}_k - \underline{g}_{k,t,i}) \tag{26}$$

$$C_i = \underline{f}_i' \sum_{k=t}^{t+N-1} (\underline{G}'_{k,t,i} \underline{V}_k^{-1} \underline{G}_{k,t,i}) \underline{f}_i \tag{27}$$

Substituting Eqs. 25 and 22 in Eq. 24, we get

$$T_i = d_i^2/C_i + \sum_{k=t}^{t+N-1} \left\{ 2(\underline{g}'_{k,t,i} \underline{V}_k^{-1} \underline{a}_k) - (\underline{g}'_{k,t,i} \underline{V}_k^{-1} \underline{g}_{k,t,i}) \right\} \tag{28}$$

The value of T_i is calculated for every vector $\underline{f}_i$ corresponding to the gross errors hypothesized. If a gross error is detected by the GED test, then the gross error that corresponds to the maximum value of T_i is identified and its magnitude is estimated by the corresponding b_i. The procedure for identifying a gross error by making use of the generalized likelihood ratio is referred to as the GLR method.

Usually, a test based on the generalized likelihood ratio (Willsky and Jones, 1974; Narasimhan and Mah, 1987) is used to detect the presence of gross errors. However, in our case there is a difficulty in using the GLR test to detect gross errors. We show in appendix B that the signature vector for controller failures is not equal to $\underline{0}$. This makes it difficult to obtain the distribution of the generalized likelihood ratio. Therefore, as described before, we use the GED test for detecting whether or not a gross error is present.

Estimating the time of occurrence of a gross error

We have shown how the signature matrices and vectors can be computed if we know the time, t, at which the gross error occurs. One possible method of estimating t is to treat it as yet another parameter to be estimated by the GLR method. In other words, we compute the likelihood ratios for every hypothesized time t (t less than or equal to k), and for every hypothesized gross error vector $\underline{f}_i$. The time, $\hat{t}$, at which the maximum likelihood ratio is obtained is estimated to be the occurrence time of the gross error. This approach was taken by Willsky and Jones (1974). Since the likelihood ratio is computed for every combination of time t and gross error vector $\underline{f}_i$, this approach is computationally cumbersome. Willsky and Jones attempted to reduce the computation by restricting t to vary over a fixed interval of time. We propose a different method for estimating the time of occurrence of the gross error, one that requires less computation. For this purpose, we make use of a simple statistical test as follows.

The innovation, $\underline{a}_k$, is normally distributed with expected values and covariance matrix given by Eqs. 11 and 12, respectively, when no gross error is present. Therefore, we can choose as a test statistic

$$\tau = (\underline{a}_k)'(\underline{H}_k \underline{P}_{k|k-1} \underline{H}_k' + \underline{Q}_k)^{-1}(\underline{a}_k) \tag{29}$$

It can be easily shown that under H_0, τ is a central chi-square variable with n degrees of freedom (Newman, 1982). We can compare τ with a chosen criterion $\chi^2_{n,1-\alpha_t}$ for any given level of significance α_t, and suspect a gross error to have occurred at time k if τ exceeds the criterion. We will refer to this test as the time of occurrence detection (TOD) test.

The TOD test is applied at every sampling time until it first rejects the null hypothesis, say at time $\hat{t}$. The application of the TOD test is stopped and the time $\hat{t}$ is declared to be the occurrence time of a suspected gross error. The signature matrices and vectors for the different hypothesized gross errors are calculated from time $\hat{t}$ to time $\hat{t} + N - 1$. At time $\hat{t} + N - 1$ the GED test is applied by making use of all the innovations from time $\hat{t}$ to $\hat{t} + N - 1$, in order to test whether a gross error is present and, if so, to identify it by making use of the generalized likelihood ratio. We start applying the TOD test from time $\hat{t} + N$ and repeat the above procedure. A flow chart of this procedure is shown in Figure 1.

Although the rejection by the TOD test at time $\hat{t}$ indicates that a gross error may have occurred, we do not immediately declare that a gross error is present. After N sampling periods have transpired, we apply the GED test and declare a gross error to be present only if this test is positive. Thus, the TOD test is used only to estimate the time of occurrence of a gross error and initiate the calculation of the signature matrices and vectors that are necessary for applying the GLR method. The above procedure requires less computing time, because the computation has to be performed only when the TOD test is rejected. Moreover, the signature matrices and vectors are computed only under the presumption that one or more gross errors occurred at a specific time, $\hat{t}$.

Comparison with the GLR formulation of Willsky and Jones

The major differences between the formulation used in our work and that of Willsky and Jones (1974) are as follows:

1. We have used a more general formulation of the hypothe-

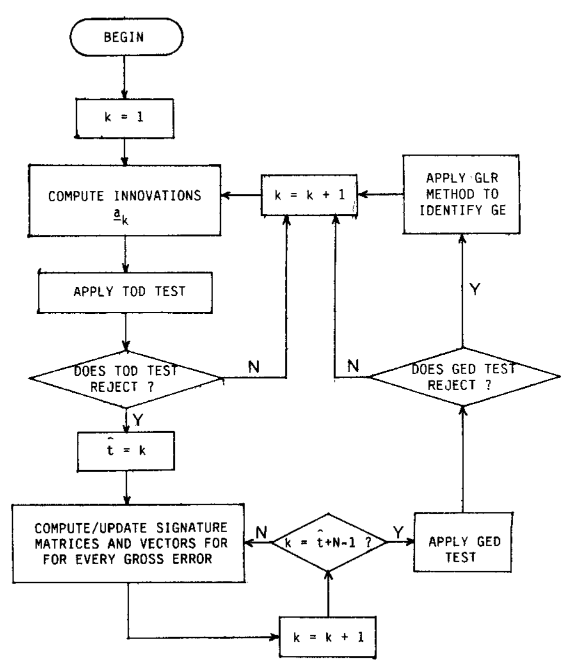

Figure 1. Flow chart of GLR method for dynamic processes.

ses. In the hypotheses used by Willsky and Jones, the signature vectors are equal to $\underline{0}$ for all the gross errors that they consider. We have seen that the signature vector for controller failures is not equal to zero and thus our generalization is necessary.

2. It is more appropriate, at least in chemical processes, to model the control inputs as a function of the measurements or estimates. We have chosen a control law based on estimates. In this case, if a controller failure is present, it is difficult to obtain the joint unconditional density of innovations. However, the joint conditional density of innovations can be obtained easily, since the innovations are serially independent when conditional statistical properties are considered, and this allows us to use the GLR method for identifying gross errors. In the work by Willsky and Jones no distinction is made between the use of conditional or unconditional statistical properties of innovations, since the control inputs are taken as known constants.

3. We estimate the time of occurrence of the gross error using the TOD test rather than by using the GLR method, which is computationally burdensome.

4. Willsky and Jones have used the GLR as the test statistic, since the signature vectors are all equal to $\underline{0}$ in their method. We use the GED test to detect the presence of a gross error, which is based on the test statistic defined by Eq. 19, while the GLR is used only to identify the gross error.

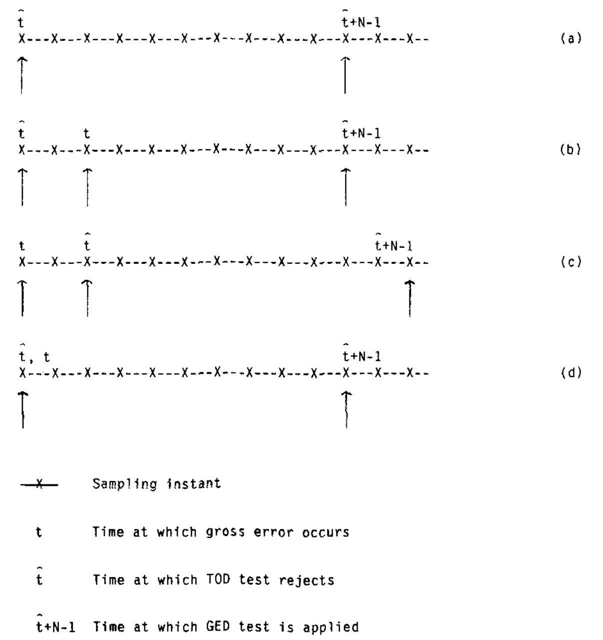

Figure 2. Different scenarios in application of GLR method.

Effect of Parameters on the Performance of the GLR Method

Performance measures

We use four measures to evaluate the performance of the GLR method. The first measure evaluates the performance of the GLR method when no gross error is present. In such cases, the GLR method may occasionally mispredict the presence of a gross error. Such a misprediction is known as a type I error. ATTI is the average time interval between two successive type I errors committed by the GLR method. The remaining three measures are used to evaluate the performance of the GLR method when gross errors are present. PGI is the proportion of gross errors that are correctly detected and identified. Even if gross errors are correctly identified, a certain time may have elapsed before their successful identification. The average time elapsed before gross errors are successfully identified (ATCI) is a measure of how quickly gross errors are identified. A final useful measure is the average relative percentage error in the estimate of gross errors that are correctly identified (AEE).

Effect of parameters

In order to apply the GLR method, the parameters that have to be chosen are:

- The level of significance of the TOD test, α_t
- The delay time for identification, N
- The level of significance of the GED test, α_g

The performance of the GLR method in the absence and presence of gross errors is affected by these parameters.

Delay Time for Identification. As N increases, the GLR method is applied less frequently. This has the advantage of increasing ATTI, the time between type I errors, but has the disadvantage of increasing ATCI, the time elapsed before a gross error is correctly identified. On the other hand, as N increases more innovations are used in the GLR method and this enables more gross errors to be correctly identified, thus increasing PGI.

Level of Significance of TOD Test. Figure 2 shows pictorially four possible cases that may occur in the application of the GLR method. Figure 2a shows the case with no gross errors present. Therefore, in this case, the TOD test has committed a type I error. In Figure 2b we depict a case in which a gross error occurs in the time interval N, after the TOD test is rejected, but before the GED test is applied. This represents a case in which the estimated time of occurrence of the gross error is less than the time at which it actually occurs. The opposite is true in the case shown in Figure 2c. Here the TOD test is rejected after the gross error has occurred, and therefore, the estimated time of occurrence of the gross error is greater than the actual time at which the gross error occurs. In the last case, Figure 2d, the time of occurrence of the gross error is estimated correctly.

An increase in the value of α_t increases the probability that the TOD test rejects, whether a gross error is present or not. This increases the number of cases shown in Figures 2a and 2b. On the other hand, if α_t decreases then the probability that the TOD test rejects decreases. This decreases the number of cases shown in Figure 2a. Moreover, since the TOD test has less power to detect the occurrence of a gross error, the number of cases corresponding to Figure 2c increases. Since we cannot predict the effect of an increase in the number of cases, corresponding to Figures 2b and 2c, on the performance of the GLR method, we conduct simulation studies that enable us to estimate their effects and choose an appropriate value of α_t.

Level of Significance of the GED Test. The GED test is used to detect the presence of gross errors. An increase in the level of significance of the GED test increases the probability of detecting a gross error. This increases the probability of making a type I error if no gross errors are present, but also increases the power to detect a gross error if it is present. These effects of the level of significance on the power and probability of type I error are typical of every statistical test.

Simulation Results and Discussion

Simulation procedure

For the purpose of these simulation studies, we consider a process with constant system matrices. A process model as described by Eqs. 1, 2, and 3; constant covariance matrices $\underline{Q}$ and $\underline{R}$, initial values of the state variables, initial estimates of the state variables that satisfy Eqs. 5M 1–12, and the covariance matrix of errors in the estimates of state variables are assumed to be given. If no gross errors are simulated, the values of the state variables and the measurements at each time are obtained using Eqs. 1 and 3, respectively. The vectors $\underline{w}_k$ and $\underline{v}_k$ are obtained by generating random errors from the multivariate normal distribution with mean $\underline{0}$ and covariance matrices $\underline{R}$ and $\underline{Q}$, respectively. The Kalman filter is used to obtain the estimates of the state vector and error covariance matrix. The control inputs are then obtained at each time using Eq. 2. If a gross error of magnitude b due to a leak, measurement bias, controller bias, or controller failure is generated at time t, then the values of the state variables, measurements, and control inputs are generated at time t and subsequent times by using the appropriate gross error model corresponding to the gross error that is generated, as given by Eqs. 4 to 8. All our simulation studies are based on a level control process described in appendix A.

Simulation of a fixed gross error

We first investigate the performance of the GLR method for different values of N, the delay time for identification, when the time of occurrence of the gross error is always estimated correctly. For this purpose, we employ a simulation scheme in which N measurements are generated in each simulation trial. A single specified gross error of given magnitude is generated at the beginning of time 1 in each simulation trial. The level of significance of the TOD test is taken to be equal to 1.0, to ensure that the TOD test always rejects at time 1. The GED test is applied at the end of N measurements to detect whether any gross error is present and if so to identify it by making use of the GLR method. This simulation trial is stopped after each application of the GLR method regardless of whether a gross error is detected by the GED test or not, and a new simulation trial is made. A simulation run consists of 10,000 simulation trials. For each simulation run the performance measures previously described are computed. We use this simulation to study the performance of the GLR method to identify each specified gross error, for different values of N. The results of this simulation, which are described in Supplementary Material 3, show that by choosing a value of N equal to 10, more than 60% of the gross errors of magnitudes between 5 and 10% of the full scale are identified. This value of N is used in all subsequent simulation runs.

Sequential simulation

The simulation scheme we describe in this section is used to evaluate the performance of the GLR method when it is continually applied to an operating process. This simulation scheme differs from the simulation of a fixed gross error in the way the GLR method is applied and in the procedure used for generating gross errors.

The application of the GLR method is as follows. Starting at time 0, measurements are generated at each time as detailed in the simulation procedure section. The GLR method as shown in Figure 1 is applied until it detects and identifies a gross error for the first time, say at time k. The sequence of measurements from time 0 to time k constitutes a simulation trial. Each simulation trial ends immediately after a gross error is detected and identified, and a new simulation trial begins. A simulation run consists of 10,000 simulation trials. Note that the length of a simulation trial is not a constant and may vary from one trial to the next.

Table 1. Range of Magnitudes of Gross Errors Used in Sequential Simulation

Gross Error	Magnitude Upper Limit	Magnitude Lower Limit
Leak in tank	−495.0	−990.0
Bias in measurement 1	0.2	0.1
Bias in measurement 2	0.70	0.35
Bias in control valve	0.127	0.0635
Failure of control valve	0.127	0.0635

We allow at most one gross error to be present in a simulation trial. At each time in a simulation trial a gross error is randomly generated according to the given probability, p_i, associated with the occurrence of gross error i. Thus, if a gross error is generated at any time, no other gross errors are generated at subsequent times in the same trial. The magnitude of a gross error generated is also randomly chosen by a uniform random number between specified lower and upper limits.

Several simulation runs were made for the level control process described in appendix A. The parameters that are varied from one run to another are p_i's and α_t. The value of N is chosen equal to 10 for all simulation runs and α_g is chosen equal to 0.1. The gross errors hypothesized and the upper and lower bounds on their random magnitudes are shown in Table 1. For simplicity, we have chosen the value of p_i to be the same for all gross errors. We have also chosen p_i to be a constant at all times. The results of our simulation are presented in Tables 2 and 3. The simulation runs listed in Table 2 are made with p_i's chosen equal to 0.01 for all gross errors, and for the runs in Table 3, p_i's are chosen equal to 0.001.

In Tables 2 and 3, the levels of significance of the TOD test used for the four runs are 0.05, 0.25, 0.5 and 1.0, respectively, as shown in column 2. These values are chosen to cover the range of possible values from 0 to 1. The number of gross errors generated, which is shown in column 3, can be observed to increase with p_i as expected. The following observations can be made from the performance measures listed in columns 4 through 7 of Tables 2 and 3:

1. From column 4 it is observed that there is an increase of

Table 2. Results of Sequential Simulation for $p_i = 0.01$

Run No.	α_t	No. Gross Errors Generated	PGI	ATCI	ATTI	AEE %
1.4a	0.05	8,797	0.79	11.0	24.8	21.5
1.4b	0.25	8,344	0.69	9.3	22.2	24.2
1.4c	0.50	8,436	0.66	9.4	21.9	25.2
1.4d	1.0	8,688	0.63	9.3	22.6	26.2

Table 3. Results of Sequential Simulation for $p_i = 0.001$

Run No.	α_t	No. Gross Errors Generated	PGI	ATCI	ATTI	AEE %
1.5a	0.05	3,282	0.78	11.1	67.5	22.5
1.5b	0.25	2,711	0.67	9.4	54.8	25.3
1.5c	0.50	2,938	0.65	8.9	59.8	25.9
1.5d	1.0	3,409	0.62	9.8	69.2	27.8

14–16% in the proportion of gross errors identified as α_t decreases from 1.0 to 0.05.

2. Column 5 shows that ATCI is highest for $\alpha_t = 0.05$, but is only marginally higher ($\simeq$2.0) than those obtained for other values of α_t. A low value of ATCI is desirable since this implies that gross errors will be identified quickly.

3. A high value of ATTI is desired since this decreases the frequency of type I errors. From column 6 it is observed that the value of ATTI is maximum when $\alpha_t = 0.05$, Table 2, or close to the maximum value, Table 3.

4. The last column shows that the least error in the estimate of gross errors is obtained for $\alpha_t = 0.05$.

From the above observations we infer that $\alpha_t = 0.05$ is the best choice. This choice will give a marginally higher value for ATCI, but improvements in all other performance measures are obtained. In the section on the effect of parameters we pointed out that a low value of α_t increases the number of cases shown in Figure 2c. Therefore, from the results of our simulation we can infer that the GLR method performs better if $\hat{t}$ is greater than t, Figure 2c, as compared to cases when $\hat{t}$ is less than t, Figure 2b. This also seems intuitively reasonable, since in the case of Figure 2c all the innovations used in the GLR method contain the effect of the gross error, but in the case of Figure 2b only some of the innovations contain the effect of the gross error. This type of simulation study can be utilized for choosing an appropriate value of α_t when applying the GLR method to other processes.

Conclusions

In this paper we have developed the methodology for identifying gross errors in closed-loop dynamic processes. We have shown that by exploiting the conditional statistical properties of innovations, gross errors caused by failure of controllers can also be identified. We also performed simulation studies to guide the selection of the delay time for gross error identification and the level of significance of the TOD test. In the system we simulated, magnitudes of gross errors between 5 and 10% of full scale are identified with probabilities greater than 0.6 within 10 sampling periods from the occurrence of gross errors. Sequential simulation studies also show that a low value of the level of significance of the TOD test leads to better overall performance.

Control laws based on the estimates of state variables are used in our work. The GLR method is also applicable for conventional linear control laws based on the measured values of variables. For this purpose, the equations for calculating the signature matrices and signature vectors of gross errors must be appropriately modified. There is a certain amount of analytical labor involved in these calculations. However, such a complete description of the effect of a gross error on all the measurements cannot be obtained from a qualitative reasoning such as "signed digraphs" used by other workers (Kramer, 1987).

In this paper, we have demonstrated the applicability of the GLR method for identifying four types of gross error. There exists a need for better understanding of other types of gross errors, such as pipe blockages and fouling of heat exchangers, that commonly occur and for improved modeling of these errors.

Finally, an important issue to be examined in future research is the robustness of the GLR method when differences exist between the true process model and the linear process model that is used, and when nonlinearities are present in the process.

Acknowledgment

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Notation

$\underline{a}_k$ = vector of innovations at time k
$\underline{a}_k^1$ = part of $\underline{a}_k$ due to random errrors only
$\underline{a}_k^2$ = part of $\underline{a}_k$ due to gross error only
$\underline{A}_k$ = state transition matrix at time k
b = magnitude of gross error
b_i = magnitude of gross error i
$\hat{b}_i$ = estimated magnitude of gross error i
$\underline{B}_k$ = input matrix at time k in dynamic process model
C_i = quantity, Eq. 27
$\underline{C}_k$ = control matrix at time k
d_i = quantity, Eq. 26
$\underline{e}_i$ = ith unit vector
$\underline{f}_i$ = gross error vector for gross error i
$\underline{G}_{k,t,i}$ = signature matrix at time k for gross error i that occurs at time t
$\underline{g}_{k,t,i}$ = signature vector at time k for gross error i that occurs at time i
h = number of gross errors hypothesized
H_0 = null hypothesis
H_1 = alternative hypothesis
$\underline{H}_k$ = measurement matrix at time k
$\underline{I}$ = identity matrix
$\underline{J}_{k,t,i}$ = matrix, Eq. B20
$\underline{j}_{k,t,i}$ = vector, Eq. B21
$\underline{K}_k$ = Kalman gain matrix
m = number of control inputs in dynamic model
$\underline{m}_i$ = gross error vector for leak in unit i (discrete model)
$\underline{m}_i^*$ = gross error vector for leak in unit i (continous model)
n = number of measurements
N = delay time for identification; number of innovations used in GLR method
p = dimension of process noise vector
p_i = probability of occurrence of gross error i
$\underline{P}_{k|k-1}$ = conditional covariance matrix of state estimate error at time k, given measurements up to time $k - 1$
$\underline{P}_{k|k}$ = conditional covariance matrix of state estimate error at time k, given measurements up to time k
q = number of process units
$\underline{Q}_k$ = covariance matrix of measurement errors at time k
$\underline{R}_k$ = covariance matrix of process noise at time k
s = number of state variables
$\underline{S}_k$ = matrix at time k, Eq. B12
$\underline{t}_{k,t,i}$ = vector, Eq. B14
T_i = generalized likelihood ratio for gross error i
T = maximum generalized likelihood ratio
$\underline{T}_{k,t,i}$ = matrix, Eq. B13
$\underline{u}_k$ = control inputs at time i
$\underline{u}_k^1$ = part of $\underline{u}_k$ due to random errors only
$\underline{u}_k^2$ = part of $\underline{u}_k$ due to gross error only
$\underline{v}$ = vector of measurement errors
$\underline{V}_k$ = covariance matrix of innovations
$\underline{w}_k$ = process noise vector at time k
$\underline{x}_k$ = vector of true values of state variables
$\underline{x}_k^1$ = part of $\underline{u}_k$ due to random errors only
$\underline{x}_k^2$ = part of $\underline{u}_k$ due to gross error only

$\hat{\underline{x}}_{k|k-1}$ – conditional estimates at time k of state variables, given measurements up to time $k-1$

$\hat{\underline{x}}_{k|k}$ – conditional estimates at time k of state variables, given measurements up to time k

$\hat{\underline{x}}^1_{k|k}$ – part of $\hat{\underline{x}}_{k|k}$ due to random errors only

$\hat{\underline{x}}^2_{k|k}$ – part of $\hat{\underline{x}}_{k|k}$ due to gross error only

$\underline{X}$ – set of vectors used in GLR method

$\underline{z}_k$ – measurement vector at time k

$\underline{z}^1_k$ – part of $\underline{z}_k$ due to random errors only

$\underline{z}^2_k$ – part of $\underline{z}_k$ due to gross error only

$\underline{Z}_k$ – set of measurement vectors $\underline{z}_j$ from 1 to time k

$\underline{0}$ – vector of matrix or zeros

Greek symbols

α_g – level of significance of GED test

α_t – level of significance of TOD test

$\underline{\Gamma}_k$ – process noise matrix in dynamic model

χ^2_n – chi-square distribution with n degrees of freedom

$\chi^2_{n,1-\alpha}$ – upper $1-\alpha$ quantile of chi-square distribution with n degrees of freedom

$\lambda_{(\cdot)}$ – likelihood ratio, Eq. 20

$\underline{\nu}_{k,t,i}$ – quantity, Eq. 22

ψ – GED test statistic

σ_{k-t} – unit step, Eq. 5

τ – TOD test statistic

Other symbols

a' – transpose of a

a^{-1} – inverse of a

cov $[a]$ – $E[(a-E[a])(a-E[a])']$

cov $[a,b]$ – $E[(a-E[a])(b-E[b])']$

$E[a]$ – expected value of a

$Pr\{a\}$ – probability of a

$Pr\{a|b\}$ – conditional probability of a, given b

Abbreviations

AEE – average relative percentage error in estimate of a gross error

ATCI – average time elapsed before a gross error is correctly identified

ATTI – average time between two successive type I errors

PGI – proportion of gross errors identified

GED – gross error detection (test)

GLR – generalized likelihood ratio

TOD – time of occurrence detection (test)

Appendix A: Level Control Process

Consider a process system of a level control (Bellingham and Lees, 1977) shown in Figure 3. The derivation of the linear discrete state space model for this process is described in Supplementary Material 2. The process model, assuming that a leak of magnitude b occurs in the tank, is given by

$$\begin{bmatrix} h_{k+1} \\ x_{k+1} \end{bmatrix} = \begin{bmatrix} 0.995 & -0.1373 \\ 0.00 & 1.0 \end{bmatrix} \begin{bmatrix} h_k \\ x_k \end{bmatrix} + \begin{bmatrix} 0.0 \\ 1.0 \end{bmatrix} a_k + \begin{bmatrix} 0.00012 & 0.0 \\ 0.0 & 1.0 \end{bmatrix} \begin{bmatrix} F_{3k} \\ e_k \end{bmatrix} + \begin{bmatrix} 0.00012 \\ 0.0 \end{bmatrix} b \quad (A1)$$

The control law is chosen as

$$a_k = [0.0326 \; -1.0] \; [h_k x_k]' \quad (A2)$$

and the measurement equation is given by

$$\begin{bmatrix} z_{1k} \\ z_{2k} \end{bmatrix} = \begin{bmatrix} 0.631 & 0.0 \\ 0.00 & 1.57 \end{bmatrix} \begin{bmatrix} h_k \\ x_k \end{bmatrix} + \begin{bmatrix} v_{1k} \\ v_{2k} \end{bmatrix} \quad (A3)$$

where h_k and x_k are deviations from the nominal value of the level in the tank and the value position, respectively. The control input is the adjustment to valve position a_k. The variables $\underline{F}_{3k}$ and $\underline{e}_k$ are assumed to be random process noise distributed normally with variances 62,500 and 0.0025, respectively. The variances of the measurement noises, v_{ik} and v_{2k}, are both equal to 0.01.

Note that the gross error model for a leak described by Eq. A1 corresponds to the general form of Eq. 4. The process model without any gross errors can be obtained by setting b equal to 0 in Eq. A1.

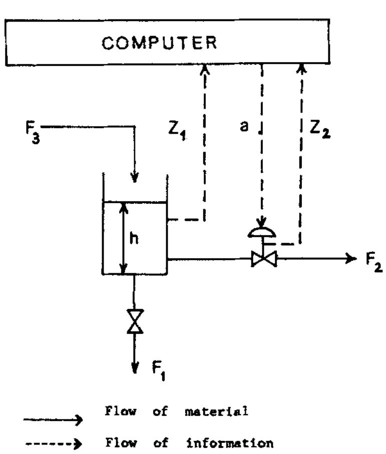

Figure 3. Level control process.

Appendix B: Computation of Signature Matrices and Vectors

Let us assume that a failure of controller i has occurred at time t. We derive the effect of this controller failure on the innovations at any time k greater than or equal to t. The true process model in the presence of a failure of controller i is given by Eqs. 1, 3, and 8. For simplicity, in the subsequent development the notation σ_{k-t} is ommitted from the gross error model, since its value is unity for all times k greater than t. The estimator equations are given by Eqs. (SM1-6) to (SM1-11), regardless of whether a gross error is present or not. Since the system model and estimator are linear, we can split the true values of state variables, the conditional state estimates, the measurements the control inputs, and the innovations into two parts as

$$\underline{x}_k = \underline{x}^1_k + \underline{x}^2_k \quad (B1)$$

$$\hat{\underline{x}}_{k|k} = \hat{\underline{x}}^1_{k|k} + \hat{\underline{x}}^2_{k|k} \quad (B2)$$

$$\underline{z}_k = \underline{z}^1_k + \underline{z}^2_k \quad (B3)$$

$$\underline{a}_k = \underline{a}^1_k + \underline{a}^2_k \quad (B4)$$

$$\underline{u}_k = \underline{u}^1_k + \underline{u}^2_k \quad (B5)$$

where $\underline{x}^1_k$, $\hat{\underline{x}}^1_{k|k}$, $\underline{z}^1_k$, $\underline{a}^1_k$, and $\underline{u}^1_k$ do not contain the effects of the gross error, and $\underline{x}^2_k$, $\hat{\underline{x}}^2_{k|k}$, $\underline{z}^2_k$, $\underline{a}^2_k$, and $\underline{u}^2_k$ are due solely to the effects of the gross error. The quantities with superscript 2 will be equal to $\underline{0}$ if there is no gross error.

We define the linear dependence of $\underline{x}_k^2$, $\hat{\underline{x}}_{k|k}^2$, $\underline{a}_k^2$ on the gross error by the following equations:

$$\underline{x}_k^2 = b\underline{T}_{k,t,i}\underline{f}_i + \underline{t}_{k,t,i} \quad \text{(B6)}$$

$$\hat{\underline{x}}_{k|k}^2 = b\underline{J}_{k,t,i}\underline{f}_i + \underline{j}_{k,t,i} \quad \text{(B7)}$$

$$\underline{a}_k^2 = b\underline{G}_{k,t,i}\underline{f}_i + \underline{g}_{k,t,i} \quad \text{(B8)}$$

The matrices and vectors defined on the righthand sides of Eqs. B6 to B8 are subscripted with three indices to indicate that these quantities depend on the time k of interest, the time t when the gross error occurred, and the type of gross error i. It should also be noted that these quantities are equal to $\underline{0}$ for time k less than t, since there is no gross error before time t. The vector $\underline{f}_i$ in Eqs. B6 to B8 depends on the type of gross error. For a failure of controller i, the vector $\underline{f}_i$ is equal to $\underline{e}_i$: $m \times 1$, as in Eq. 8. We are eventually interested in computing the matrix $\underline{G}_{k,t,i}$, which we refer to as the signature matrix, and the vector $\underline{g}_{k,t,i}$, which we refer to as the signature vector. These are computed as follows.

First we derive the recurrence equations for $\underline{T}_{k,t,i}$ and $\underline{t}_{k,t,i}$. Substituting Eqs. B1 and B5 in Eq. 1, we get

$$\underline{x}_k^1 + \underline{x}_k^2 = \underline{A}_{k-1}(\underline{x}_{k-1}^1 + \underline{x}_{k-1}^2) + \underline{B}_{k-1}(\underline{u}_{k-1}^1 + \underline{u}_{k-1}^2) + \underline{\Gamma}_{k-1}\underline{w}_{k-1} \quad \text{(B9)}$$

By definition $\underline{x}_k^2$ is due solely to the effect of the gross error. Therefore,

$$\underline{x}_k^2 = \underline{A}_{k-1}\underline{x}_{k-1}^2 + \underline{B}_{k-1}\underline{u}_{k-1}^2 \quad \text{(B10)}$$

Substituting for $\underline{x}_{k-1}^2$ and $\underline{u}_{k-1}^2$ in Eq. B10, using Eqs. B6, 8, and B7, we obtain

$$\underline{x}_k^2 = b(\underline{A}_{k-1}\underline{T}_{k-1,t,i} + \underline{S}_{k-1}\underline{J}_{k-1,t,i} + \underline{B}_{k-1})\underline{e}_i - \underline{B}_{k-1}\underline{e}_i\underline{e}_i'\underline{C}_{k-1}\hat{\underline{x}}_{k-1|k-1} + \underline{A}_{k-1}\underline{t}_{k-1,t,i} + \underline{S}_{k-1}\underline{j}_{k-1,t,i} \quad \text{(B11)}$$

where

$$\underline{S}_k = \underline{B}_k\underline{C}_k \quad \text{(B12)}$$

Note that we have used the gross error model for a controller failure, as defined by Eq. 8, in substituting for the control inputs. Comparing Eq. B11 with the definition of $\underline{T}_{k,t,i}$ and $\underline{t}_{k,t,i}$ in Eq. B6, we obtain

$$\underline{T}_{k,t,i} = \underline{A}_{k-1}\underline{T}_{k-1,t,i} + \underline{S}_{k-1}\underline{J}_{k-1,t,i} + \underline{B}_{k-1} \quad \text{(B13)}$$

$$\underline{t}_{k,t,i} = \underline{A}_{k-1}\underline{t}_{k-1,t,i} + \underline{S}_{k-1}\underline{j}_{k-1,t,i} - \underline{B}_{k-1}\underline{e}_i\underline{e}_i'\underline{C}_{k-1}\hat{\underline{x}}_{k-1|k-1} \quad \text{(B14)}$$

Next we get the recurrence relations for computing $\underline{G}_{k,t,i}$ and $\underline{g}_{k,t,i}$. Substituting for $\underline{z}_k$ and $\hat{\underline{x}}_{k|k-1}$ by using Eqs. 3 and (SM1-6), respectively, in Eq. 9 and separating the effects of the gross error, we get

$$\underline{a}_k^2 = \underline{H}_k\underline{x}_k^2 - \underline{H}_k(\underline{A}_{k-1} + \underline{S}_{k-1})\hat{\underline{x}}_{k-1|k-1}^2 \quad \text{(B15)}$$

Using Eqs. B6 and B7 in the righthand side of Eq. B15 we obtain

$$\underline{a}_k^2 = b\underline{H}_k[\underline{T}_{k,t,i} - (\underline{A}_{k-1} + \underline{S}_{k-1})\underline{J}_{k-1,t,i}]\underline{e}_i + \underline{H}_k[\underline{t}_{k,t,i} - (\underline{A}_{k-1} + \underline{S}_{k-1})\underline{j}_{k-1,t,i}] \quad \text{(B16)}$$

Comparing Eq. B16 with the definition of $\underline{G}_{k,t,i}$ and $\underline{g}_{k,t,i}$, in Eq. B8 we get

$$\underline{G}_{k,t,i} = \underline{H}_k[\underline{T}_{k,t,i} - (\underline{A}_{k-1} + \underline{S}_{k-1})\underline{J}_{k-1,t,i}] \quad \text{(B17)}$$

$$\underline{g}_{k,t,i} = \underline{H}_k[\underline{t}_{k,t,i} - (\underline{A}_{k-1} + \underline{S}_{k-1})\underline{j}_{k-1,t,i}] \quad \text{(B18)}$$

Finally we derive the recurrence relation for $\underline{J}_{k,t,i}$ and $\underline{j}_{k,t,i}$. Substituting for $\hat{\underline{x}}_{k|k-1}$ using Eq. SM1-6 and for $\underline{a}_k$ using Eq. 9 in Eq. SM1-9 and separating the effects of the gross error, we get

$$\hat{\underline{x}}_{k|k}^2 = (\underline{A}_{k-1} + \underline{S}_{k-1})\hat{\underline{x}}_{k-1|k-1}^2 + \underline{K}_k\underline{a}_k^2 \quad \text{(B19)}$$

Comparing the above equation with the definition of $\underline{J}_{k,t,i}$ and $\underline{j}_{k,t,i}$ in Eq. B7, we obtain

$$\underline{J}_{k,t,i} = (\underline{A}_{k-1} + \underline{S}_{k-1})\underline{J}_{k-1,t,i} + \underline{K}_k\underline{G}_{k,t,i} \quad \text{(B20)}$$

$$\underline{j}_{k,t,i} = (\underline{A}_{k-1} + \underline{S}_{k-1})\underline{j}_{k-1,t,i} + \underline{K}_k\underline{g}_{k,t,i} \quad \text{(B21)}$$

The signature matrix and signature vector are thus computed using Eqs. B17 and B18, respectively, which in turn requires the computation of matrices $\underline{T}_{k,t,i}$ and $\underline{J}_{k-1,t,i}$ and vectors $\underline{t}_{k,t,i}$ and $\underline{j}_{k-1,t,i}$ using Eqs. B13, B20, B14, and B21. The matrices $\underline{T}_{k,t,i}$, $\underline{G}_{k,t,i}$, and $\underline{J}_{k,t,i}$ and the vectors $\underline{t}_{k,t,i}$, $\underline{g}_{k,t,i}$, and $\underline{j}_{k,t,i}$ are all equal to $\underline{0}$ for k less than t.

The computation of the signature matrices and signature vectors for leaks, measurement biases, and controller biases proceeds along similar lines, using the appropriate gross error model for each type of gross error. In these cases, it turns out that the vectors $\underline{t}_{k,t,i}$, $\underline{g}_{k,t,i}$, and $\underline{j}_{k,t,i}$ are equal to $\underline{0}$ for all k. The same notation as in Eqs. B1 through B8 is used with the understanding that the vector $\underline{f}_i$ may be different for each type of gross error. The recurrence equations for the computation of the signature matrices are as follows.

Process leaks

If a process leak of magnitude b occurs at time t, then the true system model is given by Eqs. 2, 3, and 4. The recurrence equations for calculating the signature matrix are given by

$$\underline{T}_{k,t,i} = \underline{A}_{k-1}\underline{T}_{k-1,t,i} + \underline{S}_{k-1}\underline{J}_{k-1,t,i} + \underline{I} \quad \text{(B22)}$$

$$\underline{G}_{k,t,i} = \underline{H}_k[\underline{T}_{k,t,i} - (\underline{A}_{k-1} + \underline{S}_{k-1})\underline{J}_{k-1,t,i}] \quad \text{(B23)}$$

$$\underline{J}_{k,t,i} = (\underline{A}_{k-1} + \underline{S}_{k-1})\underline{J}_{k-1,t,i} + \underline{K}_k\underline{G}_{k,t,i} \quad \text{(B24)}$$

Measurement biases

The true system model for measurement biases is described by Eqs. 1, 2, and 6. The recurrence equations for computing the signature matrix are obtained as

$$\underline{T}_{k,t,i} = \underline{A}_{k-1}\underline{T}_{k-1,t,i} + \underline{S}_{k-1}\underline{J}_{k-1,t,i} \quad \text{(B25)}$$

$$\underline{G}_{k,t,i} = \underline{H}_k[\underline{T}_{k,t,i} - (\underline{A}_{k-1} + \underline{S}_{k-1})\underline{J}_{k-1,t,i}] + \underline{I} \quad \text{(B26)}$$

$$\underline{J}_{k,t,i} = (\underline{A}_{k-1} + \underline{S}_{k-1})\underline{J}_{k-1,t,i} + \underline{K}_k\underline{G}_{k,t,i} \quad \text{(B27)}$$

Controller biases

Using the true process model for controller biases, described by Eqs. 1, 3, and 7, the signature matrix is computed using the following recurrence equations:

$$\underline{T}_{k,t,i} = \underline{A}_{k-1}\underline{T}_{k-1,t,i} + \underline{S}_{k-1}\underline{J}_{k-1,t,i} + \underline{B}_{k-1} \quad \text{(B28)}$$

$$\underline{G}_{k,t,i} = \underline{H}_k[\underline{T}_{k,t,i} - (\underline{A}_{k-1} + \underline{S}_{k-1})\underline{J}_{k-1,t,i}] \quad \text{(B29)}$$

$$\underline{J}_{k,t,i} = (\underline{A}_{k-1} + \underline{S}_{k-1})\underline{J}_{k-1,t,i} + \underline{K}_k\underline{G}_{k,t,i} \quad \text{(B30)}$$

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