Real-time Performance Assessment of Inferential Sensors \star

Shima Khatibisepehr^{*} Biao Huang^{**} Swanand Khare^{***} Ramesh Kadali^{****}

 * Department of Chemical and Materials Engineering, University of Alberta, Edmonton, Alberta T6G 2G6, Canada (e-mail: shimak@ualberta.ca).
 ** Department of Chemical and Materials Engineering, University of Alberta, Edmonton, Alberta T6G 2G6, Canada (e-mail: biao.huang@ualberta.ca)

*** Department of Chemical and Materials Engineering, University of

Alberta, Édmonton, Alberta T6G 2G6, Canada (e-mail:

khare@ualberta.ca)

**** Suncor Energy Inc., Fort McMurray, Alberta, Canada (e-mail:

RKadali@Suncor.com)

Abstract: A data-driven Bayesian framework for real-time performance assessment of inferential sensors is proposed. The application of the proposed Bayesian solution does not depend on the identification techniques employed for inferential model development. The effectiveness of the proposed method is demonstrated through a simulation case study.

Keywords: Soft Sensor, Bayesian Inference, Reliability, Real-time Performance Assessment

1. INTRODUCTION

Real-time analysis of process quality variables constitutes an essential prerequisite for advanced monitoring and control of industrial processes. However, on-line measurement of such variables may involve difficulties due to the inadequacy of measurement techniques or low reliability of measuring devices. Therefore, there has been a growing interest in the development of inferential sensors to provide real-time estimates of quality variables based on their correlation with other process measurements. In many industrial applications, complete and comprehensive knowledge of involved processes is often not available. In such cases, inferential models are developed on the basis of first principles analysis as well as process data analysis.

In order to maintain the reliability of an inferential sensor, it is important to assess the accuracy of its on-line predictions. Model uncertainty (plausible alternative model structures/parameters) is one of the major sources of prediction uncertainty (McKay et al., 1999). In the context of process industries, deviations from design operating conditions are the main factors resulting in the model uncertainty and thus deterioration in performance of inferential sensors. In most of the classical identification methods, the objective is to minimize prediction errors pertaining to the identification data-set. Therefore, the generalization performance of the resulting inferential sensors are not guaranteed. In such cases, significant changes in the operating space in which the model has been identified would contribute to the model uncertainty.

Therefore, the conditional dependence of the reliability of inferential sensor predictions on characteristics of the input space and reliability of the empirical process model should be thoroughly assessed in order to develop an online performance measure. From the application point of view, a desired performance measure has two essential characteristics. First, it should effectively estimate any significant deterioration in the prediction performance when process operates outside the valid inferential region. Second, implementation and interpretation of a performance metric should be simple enough for practitioners to use. Therefore, designing a proper performance index is not straightforward. Although inferential sensors have been widely used in process industries, there are only a few publications providing a methodology to assess their online performance. In Nomikos and MacGregor (1995) and Vries and Braak (1995), approximate confidence intervals have been developed to assess the accuracy of PLS predictions based on the traditional statistical properties. The principal limitation of these approaches is that the internal empty regions within the identification data (*i.e.* the internal regions that do not contain any identification data points) cannot be diagnosed (Soto et al., 2011). Kaneko et al. (2010) proposed a distance-based method to quantify the relationship between applicability domains and accuracy of inferential sensor predictions. The authors discussed that a larger Euclidean distance of an observation to the center of identification data and to its nearest neighbors would indicate a lower prediction accuracy. This method suffers from two major drawbacks.

^{*} Financial support from Syncrude Canada Ltd., Suncor Energy Inc., Alberta Innovates - Technology Futures (AITF), and the Natural Sciences and Engineering Research Council of Canada in the form of Industrial Research Chair in Control of Oil Sands Processes is gratefully acknowledged.

First, variability of the input variables is not taken into account when determining the Euclidean distance from the center. Second, the different effects of input variables on the prediction uncertainty are ignored by correlating the prediction accuracy with a general distance measure. Yang et al. (2009) applied an ensemble method to evaluate the uncertainty of inferential sensor predictions. The basic idea is to repeatedly generate bootstrap samples of the identification data-set to re-estimate inferential model parameters. With this multitude of models, the model variation and the average model bias can be estimated. Depending on the identification procedure used, however, this method could be computationally intensive and would not be suited for on-line applications. Kaneko and Funatsu (2011) proposed to develop a multi-model inferential sensor based on the time difference of input variables in order to combine the information included in a set of local submodels into a global predictive model. Furthermore, the accuracy of global predictions has been estimated using empirical models describing the relationship between standard deviation of local predictions and standard deviation of prediction errors. The major problem of this method is that small variation in local predictions does not necessarily imply a small prediction error. The proposed metric only reflects the degree of similarities between the prediction performance of different models and does not contain any information about the reliability of each individual model.

To address the aforementioned issues, this paper provides a data-driven Bayesian framework for real-time performance assessment of inferential sensors. Such Bayesian frameworks utilizing discrete probability distributions have proven to be useful for a variety of fault diagnosis problems such as diesel engine fault diagnosis (Pernestål, 2007) and control loop performance diagnosis (Qi et al., 2010). The major contribution of the present work is to formulate and solve the problem of inferential sensor performance assessment under a Bayesian framework utilizing discrete probability distributions. The main focus is to characterize the effect of the operating space on the prediction accuracy in the absence of target measurements. The proposed method has the following attractive features: (1) A priori knowledge of process operation and underlying mechanisms can be easily incorporated in a Bayesian scheme so as to identify the criteria that might affect online performance of the designed inferential sensor. (2)Since probability density functions would reflect the actual data distribution, empty regions within the identification data-set can be identified. (3) Correlations between input variables are taken into account. (4) Contribution of each input variable in prediction uncertainty is studied. (5) Its application does not depend on the identification techniques employed for inferential model development. (6) Its real-time implementation is computationally efficient.

The remainder of this paper is organized as follows. The problem of real-time performance assessment of inferential sensors is explained in Section 2. In Section 3, the problem of reliability analysis of real-time predictions is rigorously formulated under a Bayesian framework. In Section 4, the effectiveness of the proposed Bayesian approach is demonstrated through a simulation case srudy. Section 5 summarizes this paper with concluding remarks.

2. PROBLEM STATEMENT

Consider a class of inferential models given by

$$\hat{y}_t = g(u_t; \Theta) \tag{1}$$

where \hat{y}_t denotes the predicted value of query variable inferred from the real-time measurements of influential process variables, $u_t = \{u_{k,t}\}_{k=1}^K$.

Evaluating the performance of an inferential sensor often amounts to analyzing the characteristics of prediction errors. Prediction error, also known as residual, is defined as the difference between the actual and predicted values of query variable. That is, $e_t = y_t - \hat{y}_t$, where y_t denotes the actual value of the query variable.

The absolute value of the prediction errors can be used to identify the events that would affect the reliability of the inferential model. Suppose that the performance of the inferential sensor at each time instant, r_t , can take R_e reliability statuses, *i.e.* $r_t \in \{r^1, ..., r^{R_e}\}$. For instance, different degrees of reliability can be assigned to the inferential sensor predictions as follows:

$$r^{j} = \begin{cases} \text{Reliable} & 0 < |e_{t}| \leq 2\sigma_{e} \\ \text{Moderately reliable} & 2\sigma_{e} < |e_{t}| \leq 3\sigma_{e} \\ \text{Unreliable} & \text{Otherwise} \end{cases}$$
(2)

where the thresholds are considered as design parameters reflecting the tolerable amount of prediction error, and need to be adjusted based on the requirements of each application.

If y_t is observed, calculation of the performance index is straightforward. During on-line implementation of an inferential sensor, however, such real-time measurements are often not available frequently and regularly. Therefore, the main challenge is to assess the reliability of the inferential sensor predictions in the absence of actual values. Mathematically, the objective is to evaluate the conditional probability mass function $f(e_t|u_t, \hat{y}_t; \sigma_e)$.

3. REAL-TIME PERFORMANCE ASSESSMENT OF INFERENTIAL SENSORS

Given the training data-set $\mathcal{D} = \{(u_t, y_t)\}_{t=1}^N$, an inferential sensor provides a real-time prediction, \hat{y}_t , on the basis of real-time measurements of k input variables, $u_t =$ $\{u_{k,t}\}_{k=1}^{K}$. It is noteworthy that the identification dataset contains both input and output measurements that are typically available from plant tests and/or historical plant operations at lower sampling frequency. Therefore, the model prediction errors within the identification dataset, $\{e_t\}_{t=1}^N$, can be directly calculated from $\{(u_t, y_t)\}_{t=1}^N$. A set of indicator variables, $\{Q_t\}_{t=1}^N = \{q_t^{u_1}, \dots, q_t^{u_k}\}_{t=1}^N \in \mathbb{R}$ $\mathbb{R}^{K \times N}$, is introduced to partition the operating space into multiple modes. Suppose that each real-time input measurement, $u_{k,t}$, can take O_{u_k} operating statuses. Prior knowledge of process operation (e.g. normal or unusualoperating conditions) can be incorporated to properly partition the operating range of each process variable as well as the operating space of a set of process variables. In the absence of a priori knowledge, statistical analysis of operational and laboratory data may guide the choice of partitions. For instance, if it can be assumed that the input variables are Gaussian distributed random variables such

that $u_k \sim \mathcal{N}(\mu_k, \sigma_k^2)$, then different operating statuses may be assigned to the input measurements as follows:

$$q_t^{u_k} = \begin{cases} \text{Normal} & 0 < |u_{k,t} - \mu_k| \le 2\sigma_k \\ \text{High} & 2\sigma_k < |u_{k,t} - \mu_k| \le 3\sigma_k \\ \text{Abnormal} & 3\sigma_k < |u_{k,t} - \mu_k| \end{cases}$$
(3)

where the thresholds are considered as design parameters chosen to provide adequate coverage of the operating space. Moreover, the generalization performance of the inferential sensor may guide the assignment of operating statuses. We would like to emphasize that our proposed method does not require any assumption about the probability density function (PDF) of input variables.

The on-line performance assessment of the inferential sensor amounts to evaluating the posterior probability distribution of r_t given the operating status of the current measured inputs with reference to the historical data. The maximum *a posteriori* (MAP) estimate of reliability status is thus obtained from the following expression:

$$\widehat{r}_t = \operatorname*{argmax}_{r_t} p(r_t | Q_t, \mathcal{D}) \tag{4}$$

Applying Baye's rule, the posterior probability of r given reliability status of the current measured inputs and output can be written as

$$p(r_t|Q_t, \mathcal{D}) = \gamma p(Q_t|r_t, \mathcal{D})p(r_t)$$
(5)

where γ is a normalizing constant.

The random variable r_t is a categorical variable and can be modelled by

$$p(r_t) = \prod_{j=1}^{R_e} p(r_t = r^j)^{[r_t = r^j]}$$
$$= \prod_{j=1}^{R_e} (\varpi_j^e)^{[r_t = r^j]}$$
(6)

where the operation $[r_t = r^j]$ evaluates to 1 if $r_t = r^j$ and evaluates to 0 otherwise.

Each input indicator variable is a random categorical variable. As a result, the vector of indicator variables Q_t is an assembly of K random categorical variables. Given the reliability status of the inferential sensor, Q_t can thus be modelled by a joint multinomial distribution with $S = \prod_{k=1}^{K} O_{u_k}$ points in its sample space (*i.e.* $Q_t \in \{Q^1, ..., Q^S\}$):

$$p(Q_t | \varpi_j^Q, r_t = r^j, \mathcal{D}) = \prod_{s=1}^{S} p(Q_t = Q^s | r_t = r^j, \mathcal{D})^{[Q_t = Q^s]}$$
$$= \prod_{s=1}^{S} (\varpi_{s|j})^{[Q_t = Q^s]}$$
(7)

where $\varpi_j^Q = \{ \varpi_{s|j} \}_{s=1}^S$ is a set of hyperparameters characterizing the likelihood function in (5).

Since the hyperparameters are typically not known *a priori*, the likelihood function is evaluated by integrating over the hyperparameters' space:

$$p(Q_t|r_t = r^j, \mathcal{D}) = \int p(Q_t|\varpi_j^Q, r_t = r^j, \mathcal{D}) \\ \times p(\varpi_j^Q|r_t = r^j, \mathcal{D}) d\varpi_j^Q \quad (8)$$

The first term in the above integral is given by (7). Besides, Bayes' rule can be applied to derive an explicit expression for the second term. Therefore, the posterior probability distribution of the hyperparameters given the identification data $\mathcal{D} = \{(Q_t, e_t)\}_{t=1}^N$ can be written as:

$$p(\varpi_j^Q | r_t = r^j, \mathcal{D}) = \xi p(\mathcal{D} | \varpi_j^Q, r_t = r^j) p(\varpi_j^Q | r_t = r^j)$$
(9)

where ξ is a normalizing constant.

The chain rule of probability theory is used to factorize the likelihood function in (9):

$$p(\mathcal{D}|\varpi_j^Q, r_t = r^j) = \prod_{t=1}^{N_j} p(Q_t | \varpi_j^Q, r_t = r^j)$$
$$= \prod_{s=1}^S \left(\varpi_{s|j} \right)^{\nu_{s|j}}$$
(10)

where $N_j = \sum_{s=1}^{S} \nu_{s|j}$ denotes the number of samples in the identification data-set for which the reliability status of inferential sensor predictions was r^j . Equation (10) holds true only if it is reasonable to assume that the indicator variables are time-wise statistically independent.

Furthermore, the following Dirichlet distribution is considered as the hyperprior in (9) to assure generality:

$$p(\varpi_j^Q | r_t = r^j) = \frac{\Gamma\left(\sum_{s=1}^S \alpha_{s|j}\right)}{\prod_{s=1}^S \Gamma(\alpha_{s|j})} \prod_{s=1}^S \left(\varpi_{s|j}\right)^{\alpha_{s|j}-1}$$
(11)

where $\{\alpha_{s|j}\}_{s=1}^{S}$ are the Dirichlet parameters specified such that $A_j = \sum_{s=1}^{S} \alpha_{s|j}$ denotes the number of prior samples for which the reliability status of inferential sensor predictions was r^j . Also, $\Gamma(x) = (x - 1)!$ for all positive integers x. The fact that the Dirichlet distribution is the conjugate prior to the multinomial distributions justifies the choice of the Dirichlet hyperprior.

Combining (9), (10) and (11), the posterior probability of the hyperparameters then becomes (DeGroot, 1970),

$$p(\varpi|r_t = r^j, \mathcal{D}) = \frac{\Gamma(A_j + N_j)}{\prod_{s=1}^S \Gamma(\alpha_{s|j} + \nu_{s|j})} \prod_{s=1}^S \varpi_{s|j}^{\nu_{s|j} + \alpha_{s|j} - 1}$$
(12)

Substituting (7) and (12) into (8), the posterior predictive distribution can be further expressed as

$$p(Q_t|r_t = r^j, \mathcal{D}) = \int \prod_{s=1}^S \left(\varpi_{s|j} \right)^{[Q_t = Q^s] + \nu_{s|j} + \alpha_{s|j} - 1} d\varpi_j^Q$$
$$\times \frac{\Gamma(A_j + N_j)}{\prod_{s=1}^S \Gamma(\alpha_{s|j} + \nu_{s|j})}$$
(13)

Hence,

$$p(Q_t = Q^d | r_t = r^j, \mathcal{D}) = \frac{\Gamma(A_j + N_j)\Gamma(\alpha_{d|j} + \nu_{d|j} + 1)}{\Gamma(A_j + N_j + 1)}$$
$$\times \frac{\prod_{s \neq d}^S \Gamma(\alpha_{s|j} + \nu_{s|j})}{\prod_{s=1}^S \Gamma(\alpha_{s|j} + \nu_{s|j})}$$
$$= \frac{\alpha_{d|j} + \nu_{d|j}}{A_j + N_j}$$
(14)

Finally, (6) and (14) can be combined to obtain an explicit expression for the posterior probability distribution of (5):



Fig. 1. PDF of absolute value of prediction errors



Fig. 2. CDF of absolute value of prediction errors

$$p(r_t = r^j | Q_t = Q^d, \mathcal{D}) = \gamma \varpi_j^e \frac{\alpha_{d|j} + \nu_{d|j}}{A_j + N_j}$$
(15)

The above posterior probability distribution can be evaluated to obtain the MAP estimates of the qualitative reliability status of the inferential sensor (see (4)). As illustrated in Fig. 1, $r_t = r^j$ implies that $b^{j-1} < |y_t - \hat{y}_t| \leq b^j$, where b^{j-1} and b^j are the lower and upper boundaries of $|e_t|$, respectively. Note that an expression similar to (15) has also been derived by Qi et al. (2010) assuming that each discrete random variable can only take two values (*e.g.* faulty and normal). In this work, however, (15) applies to multiple values of the discrete random variables.

In order to quantify the real-time performance of inferential sensors, it is proposed to associate a numerical value to each reliability status in the light of the historical probability distribution of prediction errors. Suppose that $F(\tilde{e}_t|u_t, y_t)$ denotes the cumulative distribution function (CDF) of the absolute value of prediction error, $\tilde{e}_t = |y_t - \hat{y}_t|$. As the final stage of the training process, a quantifiable measure of reliability can be defined based on the CDF of the random variable \tilde{e}_t as follows:

$$r^{j} \triangleq \frac{p(\tilde{e}_{t} > b^{j})}{p(\tilde{e}_{t} > b^{1})} = \frac{1 - F(b^{j})}{1 - F(b^{1})} \quad \text{for} \quad j = 1 \cdots R_{e} \quad (16)$$

where $p(\tilde{e}_t > b^1)$ is a normalizing constant.

Moreover, $F(b^j) = p(\tilde{e}_t < b^j)$ is the historical probability of the inferential model resulting in a prediction error smaller than b^j . Alternatively, $r^j \propto p(\tilde{e}_t > b^j)$ is the historical probability of the inferential model resulting in a prediction error greater than b^{j} . The values of r^{j} satisfy the following conditions:

$$r^1 = 1$$
 and $r^{R_e} \to 0$ as $b^{R_e} \to \infty$ (17)

where r^1 and r^{R_e} corresponds to the highest and lowest performance of the inferential sensor, respectively. To illustrate, the following reliability statuses can be specified with reference to the cumulative distribution function shown in Fig. 2:

$$r^{j} = \begin{cases} 1 & 0 < \tilde{e}_{t} \le b^{1} \\ \frac{1 - F(b^{j})}{1 - F(b^{1})} & b^{1} < \tilde{e}_{t} \le b^{j} \\ 0 & b^{Re-1} < \tilde{e}_{t} \end{cases}$$
(18)

Finally, a reliability index (RI) can be assigned to each real-time prediction such that,

$$RI_t \triangleq \mathbb{E}[r_t] = \sum_j p(r_t = r^j | Q_t = Q^d, \mathcal{D}) r^j$$
(19)

where $RI_t \in [0, 1]$.

3.1 Design Procedure

To summarize our discussion thus far, the procedure followed to design a Bayesian performance assessment framework is outlined below:

- 1. Include the prior knowledge of process operation to properly partition the operating range of each process variable as well as the operating space of a set of process variables. In the absence of relevant prior information, the operating range of the k^{th} input variable may be partitioned as follows:
 - 1.1. Approximate the CDF of the k^{th} input, $F_k(.)$, based on the identification data.
 - 1.2. Specify the operating range of each input variable as $F_k^{-1}(b) F_k^{-1}(a)$, where $a, b \in [0, 1]$ and b > a. Note that a and b are design parameters chosen based on the quality of identification data. For instance, a = 0.05 and b = 0.95 can be selected to reduce the effect of outlying observations.
 - 1.3. Decide on the number of operating statuses, O_{u_k} , to be considered.
 - 1.4. Partition the operating range of u_k into equalwidth intervals, *i.e.* the width of each interval would be equal to $(F_k^{-1}(b) - F_k^{-1}(a))/(O_{u_k} - 2)$. It should be noted that any other data-driven approach can be used to partition the operating space (see (3)).
- 2. Specify a set of indicator variables to denote the operating status of each input variable.
- 3. Calculate the model prediction errors within the identification data-set.
- 4. Specify possible reliability statuses of inferential sensor predictions by analyzing the PDF of the absolute value of prediction error (see (2)).
- 5. Assign a numeric value to each reliability status based on the CDF of the absolute value of prediction error (see (16)).
- 6. Determine the prior distribution of reliability statuses, $\{\varpi_j^e\}_{j=1}^{R_e}$, based on the expected prediction performance of the inferential sensor as well as the

misclassification costs involved in inaccurately predicting the reliability of predictions.

- 7. Determine the prior distribution of hyperparameters given the reliability status, $p(\varpi_j^Q | r_t = r^j)$, based on the explicit prior knowledge. Note that the prior information over hyperparameters can be well-represented by Dirichlet distributions (see (11)).
- 8. Characterize the posterior probability distribution of hyperparameters given the reliability status, $p(\varpi_j^Q | r_t = r^j, \mathcal{D})$ (see (12)).
- 9. Characterize the likelihood of indicator variables for each reliability status, $p(Q_t|r_t = r^j, \mathcal{D})$, by integrating over the hyperparameters' space (see (13)).
- 10. Characterize the posterior probability distribution of each reliability status, $p(r_t = r^j | Q_t, \mathcal{D})$ (see (15)).

4. CONTINUOUS FERMENTATION REACTOR SIMULATION

The governing equations of a continuous fermentation reactor (CFR) are given by (Henson and Seborg, 1997):

$$\dot{X} = -DX + \mu X \tag{20}$$

$$\dot{S} = D(S_f - S) - \frac{1}{Y_{X/S}} \mu X$$
 (21)

$$\dot{P} = -DP + (\alpha \mu + \beta)X \tag{22}$$

where specific growth rate (μ) is defined as

$$\mu = \frac{\mu_m \left(1 - \frac{P}{P_m}\right)S}{K_m + S + \frac{S^2}{K_i}}$$
(23)

Biomass concentration (X), substrate concentration (S)and product concentration (P) are state variables of the system. Dilution rate (D) and feed substrate concentration (S_f) are considered as system inputs. Moreover, cellmass yield $(Y_{X/S})$, yield parameters (α, β) , maximum specific growth rate (μ_m) , product saturation constant (P_m) , substrate saturation constant (K_m) and substrate inhibition constant (K_i) are model parameters.

The identification data was simulated using the variable settings presented in Table 1 as well as the non-linear dynamic model given by (20)-(23). Data are collected at a relatively slow sampling rate so that data can be considered at the steady-state. An empirical linear model has been identified to describe the steady-state relationship between the input variables, dilution rate and feed substrate concentration, and the output quality variable, biomass concentration. Linear models are often used for development of inferential sensors in practical applications. In this case study, however, the identified linear model may not sufficiently represent the non-linear behavior of the fermentation process over such a wide operating space. Due to the inherent structural limitations of the identified model, the inferential sensor is thus expected to exhibit a degraded prediction performance in operating regions with low densities of identification data. Therefore, it is desirable to estimate the real-time prediction performance of the inferential sensor as well.

To determine the real-time prediction performance of this inferential sensor, a set of binary indicator variables is introduced as $\{Q_t\}_{t=1}^N = \{(q_t^{u_1}, q_t^{u_2})\}_{t=1}^N \in \mathbb{R}^{2 \times N}$. Given

Table 1. A summary of the simulated variables

Description	Distribution	Unit
Dilution rate	$\mathcal{N}(0.165, 0.00045)$	hr^{-1}
Substrate concentration	$\mathcal{N}(25, 14.15)$	kg/m^3

Table 2. Parameter settings for performance assessment of the CFR inferential model

Property	Parameter Setting
No. of operating statuses of u_1	10
No. of operating statuses of u_2	10
No. of reliability statuses	3
Reliability statuses	Reliable iff
	$0 < e_t \le 1.379$
	Moderately reliable iff
	$1.379 < e_t \le 2.758$
	Unreliable iff
	$2.758 < e_t $
Prior probability	$\varpi^e = \{0.40, 0.48, 0.12\}$
No. of prior samples	A = 22
No. of training samples	N = 2000





the reliability status of the identified inferential model, the vector of quality variables Q_t has $S = 10^2$ points in its sample space. The proposed Bayesian approach is used to assess the reliability status of the predictions. The parameter settings required to design a Bayesian reliability index are presented in Table 2. The boundaries of each reliability status have been selected based on the PDF of the absolute prediction error shown in Fig. 3. Moreover, the data-driven approach recommended in Section 3.1 was applied to partition the operating range of each input variable. Table 3 shows the confusion matrix obtained based on the reliability analysis results for N = 1000test samples. The diagonal and cross-diagonal elements of the confusion matrix shown in Table 3 represent the number of predictions with correctly and incorrectly identified reliability status, respectively. The low number of incorrectly identified instances indicates that the method could effectively determine the reliability of inferential model predictions.

The entries of the confusion matrix can be used to quantify the performance of the proposed method in terms of sensitivity, precision, and accuracy (Sokolova and Lapalme, 2009). A summary of the metrics quantifying the performance of the Bayesian reliability analysis of the CFR

	Predicted Status			
	Reliable	Mod. Reliable	Unreliable	
Reliable	432	68	0	
Mod. Reliable	20	371	15	
Unreliable	0	5	89	

Table 3. Confusion matrix for the Bayesian reliability analysis of the CFR inferential model

Table 4. Pe	erformanc	e m	etrics	s for th	ne Bayesian
reliability	analysis	of	the	CFR	inferential
model					

Reliability Class	Sensitivity	Precision	Accuracy
	(%)	(%)	(%)
Reliable	86.4	95.6	91.2
Mod. Reliable	91.4	83.6	89.2
Unreliable	94.7	85.6	98.0
Total	89.2	89.2	89.2



Fig. 4. Cumulative distribution function of the absolute prediction error obtained from the CFR inferential model

inferential model is reported in Table 4. The large values of the sensitivity, precision and accuracy are indicative of the effectiveness of the proposed method.

Regardless of the distribution of prediction error, a quantifiable measure of reliability can be defined solely based on the CDF of the absolute prediction error. From the CDF shown in Fig. 4, it is evident that the prediction error does not follow a Gaussian distribution in this example. Fig. 5 shows the reliability indices assigned to the inferential sensor predictions obtained for the test data. It can be observed that smaller reliability indices are assigned to larger prediction errors.

5. CONCLUSION

In this paper, a data-driven Bayesian framework for realtime performance assessment of inferential sensors was proposed. The main focus was to characterize the effect of the operating space on the prediction reliability in the absence of target measurements. The detail of the design procedure was presented. It was shown that the application of the proposed Bayesian solution does not depend on the identification techniques employed for inferential model development. Moreover, its real-time implementation is computationally efficient and simple for practitioners to use. The effectiveness of the proposed method was demonstrated through a simulation case study.



Fig. 5. Performance assessment of the CFR inferential model

REFERENCES

- DeGroot, M. (1970). Optimal Statistical Decisions. McGraw-Hill, New York.
- Henson, M.A. and Seborg, D.E. (1997). Nonlinear Process Control. Prentice-Hall Inc., USA.
- Kaneko, H., Arakawa, M., and Funatsu, K. (2010). Applicability domains and accuracy of prediction of soft sensor models. *AIChE Journal*, 57(6), 1506–1513.
- Kaneko, H. and Funatsu, K. (2011). Improvement and estimation of prediction accuracy of soft sensor models based on time difference. In K.G. Mehrotra, C.K. Mohan, J.C. Oh, P.K. Varshney, and M. Ali (eds.), Modern Approaches in Applied Intelligence, volume 6703 of Lecture Notes in Computer Science, 115–124. Springer-Verlag, Berlin.
- McKay, M.D., Morrison, J.D., and Upton, S.C. (1999). Evaluating prediction uncertainty in simulation models. Computer Physics Communications, 117(1-2), 44–51.
- Nomikos, P. and MacGregor, J.F. (1995). Multi-way partial least squares in monitoring batch processes. *Chemo*metrics and Intelligent Laboratory Systems, 30(1), 97– 108.
- Pernestål, A. (2007). A Bayesian Approach To Fault Isolation With Application To Diesel Engine Diagnose. Ph.D. thesis, KTH School of Electrical Engineering, Stockholm, Sweden.
- Qi, F., Huang, B., and Tamayo, E.C. (2010). Datadriven Bayesian approach for control loop diagnosis with missing data. *AIChE Journal*, 56(1), 179–195.
- Sokolova, M. and Lapalme, G. (2009). A systematic analysis of performance measures for classification tasks. *Information Processing and Management*, 45(4), 427– 437.
- Soto, A.J., Vazquez, G.E., Strickert, M., and Ponzoni, I. (2011). Target-driven subspace mapping methods and their applicability domain estimation. *Chemometrics* and Intelligent Laboratory Systems, 30(9), 779–789.
- Vries, S.D. and Braak, C.J.F.T. (1995). Prediction error in partial least squares regression: A critique on the deviation used in the unscrambler. *Chemometrics and Intelligent Laboratory Systems*, 30(2), 239–245.
- Yang, H.Y., Lee, S.H., and Na, M.G. (2009). Monitoring and uncertainty analysis of feedwater flow rate using data-based modeling methods. *IEEE Transactions on Nuclear Science*, 56(4), 2426–2433.