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A probabilistic framework for real-time performance assessment of inferential sensors ☆

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A B S T R A C T

A definition for the reliability of inferential sensor predictions is provided. A data-driven Bayesian framework for real-time performance assessment of inferential sensors is proposed. The main focus is on characterizing the effect of operating space on the reliability of inferential sensor predictions. A holistic, quantitative measure of the reliability of the inferential sensor predictions is introduced. A methodology is provided to define objective prior probabilities over plausible classes of reliability based on the total misclassification cost. The real-time performance assessment of multi-model inferential sensors is also discussed. The application of the method does not depend on the identification techniques employed for model development. Furthermore, on-line implementation of the method is computationally efficient. The effectiveness of the method is demonstrated through simulation and industrial case studies.

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 the 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 (Khatibisepehr, Huang, & Khare, 2013). Model uncertainty (plausible alternative model structures and/or parameters) is one of the major sources of prediction uncertainty (McKay, Morrison, & Upton, 1999). In the context of process industries, deviations from design operating conditions are the main factors resulting in model uncertainty and thus deterioration in the 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 is not guaranteed. In such cases, significant changes in the operating space in which the model has been identified would contribute to 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 on-line performance measure. From an 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 be used by practitioners. 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 on-line performance. In Nomikos and MacGregor (1995) and Vries and Braak (1995), approximate confidence intervals have been developed to assess the accuracy of partial least squares (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,

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Vazquez, Strickert, & Ponzoni, 2011). To monitor the performance of PLS-based inferential sensors in a real-time manner, Kamohara et al. (2004) used a multivariate statistical process control (MSPC) technique based on Hotellings T^2. The T^2 thresholds are set based on the restrictive assumption that the process and/or latent variables follow a multivariate Gaussian distribution. Kaneko, Arakawa, and Funatsu (2010) proposed a distance-based method to quantify the relationship between the applicability domains and the 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. Application of this method suffers from two major drawbacks. First, variability of the input variables is not accounted for when determining the Euclidean distance from the center. Second, the different effects of input variables on the prediction uncertainty are ignored while correlating the prediction accuracy with a general distance measure. Yang, Lee, and Na (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 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 sub-models into a global predictive model. Furthermore, the accuracy of global predictions has been estimated using empirical models describing the relationship between the standard deviation of local predictions and that of the prediction errors. Contrary to the method's assumption, 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 for the first time. The main focus is on characterizing the effect of the operating space on the prediction accuracy in the absence of target measurements. Such Bayesian frameworks utilizing discrete probability distributions have proven to be useful for a variety of fault diagnosis problems such as root cause diagnosis of process variations (Dey & Stori, 2005), diesel engine fault diagnosis (Pernestål, 2007), and control loop performance diagnosis (Qi, Huang, & Tamayo, 2010). The basic idea behind the methods proposed in the literature is to collect and synthesize information from different monitoring components to pinpoint and isolate possible sources of abnormality (Alaeddini & Dogan, 2011; Dey & Stori, 2005; Mehranbod, Soroush, & Panjapornpon, 2005; Pernestål, 2007; Qi et al., 2010; Weidl, Madsen, & Israelson, 2005). All monitoring components are assumed to take discrete values; therefore, continuous variables need to be discretized. Bayesian diagnosis frameworks are thus designed to represent conditional probabilistic relationships between discrete variables in the system being monitored. In such applications, the possible discrete values that each component can take (*e.g.* sticky/non-sticky control valves) and the set of system behavioral modes (*e.g.* normal/abnormal operation) are well-defined and have physical interpretations. Furthermore, the prior probabilities over the behavioral modes of the system are assumed to be known from the background information. However, there is no well-established, universal definition of the reliability of the inferential sensor predictions. Consequently, subjective prior knowledge of the plausible modes of reliability is not available. Moreover, discretization of continuous variables may incur an information loss, since the data falling in the same operating mode would become indistinguishable. In addition, a larger identification data-set is required to train the Bayesian framework as the resolution of the discretization increases. Since it is often not required to provide a quantitative measure of the system behavior for monitoring and diagnosis purposes, another shortcoming of the existing Bayesian monitoring methods is that they only provide maximum *a posteriori* (MAP) estimates of the behavioral mode of the system under diagnosis. However, in order to quantify the real-time performance of an inferential sensor, it is desired to provide a quantitative measure of the reliability of the inferential sensor predictions.

In a recent work (Khatibisepehr, Huang, Khare, & Kadali, 2013) presented in 10th IFAC International Symposium on Dynamics and Control of Process Systems (DYCOPS), we introduced a definition of the reliability of inferential sensor predictions and provided a methodology to discretize continuous input variables into virtual operating ranges. A Bayesian performance assessment framework was also proposed to capture conditional dependence of the reliability of inferential sensor predictions on the characteristics of the input space and the reliability of the empirical process model. The developed Bayesian framework only accommodates discrete operating statuses of inferential sensor inputs. The effectiveness of the method was demonstrated through a simulation case study. The major contributions of the present work are as follows: (1) The problem of inferential sensor performance assessment is formulated and solved under a Bayesian framework utilizing both discrete and continuous probability distributions. (2) The proposed framework is further extended for real-time performance assessment of multi-model inferential sensors. (3) A holistic, quantitative measure of the reliability of the inferential sensor predictions is introduced in order to quantify the real-time performance of inferential sensors. (4) A methodology is provided to define objective prior probabilities over plausible classes of reliability based on the misclassification cost associated with each reliability status.

The proposed Bayesian performance assessment framework has the following attractive features: (1) *A priori* knowledge of process operation and underlying mechanisms can be easily incorporated in a Bayesian scheme in order to identify the criteria that might affect the on-line 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 accounted for. (4) The contribution of each input variable to prediction uncertainty is determined. (5) Application of the method does not depend on the identification techniques employed for inferential model development. (6) Its real-time implementation is computationally efficient.

The balance of this paper is organized as follows. The problem of real-time performance assessment of inferential sensors is explained in Section 2. A general definition of the reliability of inferential sensor predictions is presented in Section 3. In Section 4, the problem of reliability analysis of real-time predictions is rigorously formulated under a Bayesian framework for single-model inferential sensors. First, the Bayesian solution for discrete operating statuses is briefly reviewed. Next, the details of the Bayesian solution for continuous operating statuses are presented. The real-time performance assessment of multi-model inferential sensors is discussed in Section 5. A simulated continuous fermentation reactor is considered in Section 6 to outline the ideas and illustrate the design procedure of the proposed method. In Section 7, the effectiveness of the proposed Bayesian approach is demonstrated through industrial case studies; the developed methodology is applied to performance assessment of two industrial inferential