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Comparison of stochastic fault detection and classification algorithms for nonlinear chemical processes

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ABSTRACT

This paper presents a comparative study of two methods to identify and classify intermittent stochastic faults occurring in a dynamic nonlinear chemical process. The methods are based on two popular stochastic modelling techniques, i.e., generalized polynomial chaos expansion (gPC) and Gaussian Process (GP). The goal is to assess which method is more efficient for fault detection and diagnosis (FDD) when using models with parametric uncertainty, and to show the capabilities and drawbacks of each method. The first method is based on a first-principle model combined with a gPC expansion to represent the uncertainty. Resulting statistics such as probability density functions (PDFs) of the measured variables is further used to infer the intermittent faults. For the second method, a GP model is used to project multiple inputs into a univariate model response from which the fault can be identified based on a minimum distance criterion. The performance of the proposed FDD algorithms is illustrated through two examples: (i) a chemical process involving two continuous, stirred tank reactors (CSTRs) and a flash tank separator, and (ii) the Tennessee Eastman benchmark problem.

1. Introduction

Early detection of abnormal events and malfunctions or faults is of great interest, since faults may affect the product quality and lead to economic losses (Gerlter, 1998). When the fault is detectable, the fault detection and diagnosis (FDD) algorithm will provide symptomatic fingerprints, which can be used by the FDD scheme to identify the root cause of the anomalous behaviour. Fault diagnosis and fault classification are used interchangeably in this work. Most of the available fault diagnosis algorithms can be broadly classified into three main classes (Isermann, 2005; Venkatasubramanian et al., 2003): (i) Analytical methods that are solely based on a first-principle model of a process; (ii) Empirical models that use the historical process data; and (iii) Semi-empirical algorithms that combine the first-principles and empirical models.

Each of these modelling approaches has its own advantages and disadvantages depending on the specific problem (Isermann, 2006), but it is recognized that while empirical models are easier to formulate and employ, first-principles models have superior extrapolation ability. The first-principles model based algorithms are developed using the physical laws that describe the dynamic behaviour of the monitored system. These algorithms typically rely on two steps: (i) residual generation obtained from the differences of model predictions and data, and (ii) residual evaluation for decision-making. The residual is often generated with either an observer for deterministic models (Patton and Chen, 1997) or a filter for stochastic process (Alrowaie et al., 2012). As an alternative of the first-principles-based FDD algorithms, multivariate statistical process monitoring techniques such as principal component analysis (PCA) have been used to extract variable correlations from data, to reduce dimensionality, and to identify faults in a process (Chiang et al., 2001). In addition, machine-learning techniques such as support vector machine have been explored to address complex process monitoring problems (Chiang et al., 2004).

Uncertainty is a major challenge for accurate fault detection and classification, since most of the FDD schemes are invariably based on models that involve imprecision (Venkatasubramanian et al., 2003). Such uncertainty may originate from either intrinsic time varying phenomena that is not considered by the model, or may arise from inaccurate calibration due to variation and noise in the data used for model calibration. However, the procedure for quantifying and propagating the effect of uncertainty on model predictions is typically omitted in reported FDD studies, leading to a loss of useful information resulting from these uncertainties

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(Patton et al., 2010). Moreover, most of the monitoring techniques in the literature are based on the point estimate to infer the faults (Isermann, 2005). Since faults and uncertainty occurring in a process may be of a stochastic nature, relying only on point estimates may not be accurate. Accordingly, it also is useful to provide information about the probability for the occurrence of faults.

To evaluate the effect of uncertainty on a first-principle model-based FDD algorithm, one option is to propagate the uncertainty onto the measured quantities used for FDD by Monte Carlo (MC) simulations (Harrison, 2010). This step often involves drawing a large number of samples and running the models with each of these samples. Thus, MC simulations may be computationally prohibitive especially for complex processes (Du et al., 2015a). On the other hand, assessing the effect of uncertainty on empirical model based algorithms, a large number of measurements are required to capture the relevant process behaviour since the calibration of the empirical model is sensitive to the amount and density of data. This may be impractical and expensive since some measurements may have little effect on the model calibration. Thus, it is useful to develop criteria for calibrating empirical models with informative measurements that are sensitive to both faults and uncertainties.

To improve the computational efficiency and accuracy of model calibration, this paper presents and compares two FDD algorithms to account for uncertainty. The faults in this current work are stochastic perturbations superimposed on intermittent step changes (or mean values) in specific input variables of a nonlinear chemical plant. In contrast with work in the literature (Tong et al., 2013), the process is assumed to operate at multiple operating modes associated with process changeovers. Each operating mode is defined by the mean value of a specific input variable. One mode or mean value denotes the normal operating condition and the other mean values represent faulty conditions. Further, it is assumed that faults may occur intermittently (Eriksson et al., 2013), i.e., the process can switch between faulty and normal operating conditions. The stochastic perturbations around the mean values are common occurrence in processes generally due to materials variability or imperfect control. The changes among different mean values are generally not stochastic since they are very often initiated by plant operators. However, in this work they were considered stochastic only for the purpose of assessing performance of the proposed algorithms in an unbiased fashion, i.e., to avoid obtaining results that are specific for a particular choice of the time changes between mean values.

For uncertainty quantification, two popular stochastic modelling techniques are used in this work, i.e., generalized polynomial chaos (gPC) and Gaussian Process (GP). For the first FDD method, gPC model (Ghanem and Spanos, 1991; Xiu, 2010) in combination with a first-principles model is developed to quantify and propagate the uncertainty onto the measured quantities that can be used for fault detection. For the second method, an empirical-model is developed with a GP approach (Rasmussen and Williams, 2006), which predicts the mean and variance of faults simultaneously. In this work, the variance is used to calibrate the GP model with a model adjustment method, and the mean is used to infer faults through a minimum disturbance criterion.

The objective in this work is to address the respective capabilities and limitations of these methods and investigate the possibility to overcome these limitations by combining both algorithms. For this purpose, the performance of each FDD method is evaluated in terms of fault classification rate of input faults that consist of stochastic perturbations superimposed on intermittently changing mean values of the input faults. The goal is to identify and detect these mean value changes using available measurements corrupted with noise in the presence of random perturbations around each mean value of faults.

In summary, the contributions in this current work are: (i) the development and use, in the context of fault detection and diagnosis, of gPC models-based and GP models-based FDD algorithms. (ii) The comparison of first-principles model-based (gPC) and empirical model-based (GP) methods for the detection of faults. (iii) The development of a normal cumulative distribution function-based model adjustment method for the GP model calibration.

This paper is organized as follows. In Section 2, the formulation of a fault detection problem is presented followed by the theoretical background of the gPC and GP theories. The fault detection and diagnosis (FDD) algorithms are explained in Section 3. A nonlinear chemical plant involving two continuously stirred tank reactors and a flash tank separator and the Tennessee Eastman challenge problem are introduced as examples in Section 4. Analysis and discussion of the results are given in Section 5 followed by conclusions in Section 6.

2. Problem formulation and theoretical background

2.1. Formulation of unknown stochastic faults

A process subjected to stochastic parametric input faults can be described by a set of nonlinear ordinary differential equations (ODEs) as follows:

$$\begin{aligned} &\dot{\boldsymbol{x}} = f(t, \boldsymbol{x}, \mathbf{u}; \mathbf{g}) + \boldsymbol{v} \\ &0 \le t \le t_f, \boldsymbol{x}(0) = \boldsymbol{x}_0 \end{aligned}, \tag{1}$$

where the vector $\boldsymbol{x} \in \boldsymbol{R}^n$ represent the system states (measured quantities) with initial conditions $\boldsymbol{x}_0 \in \boldsymbol{R}^n$ over time domain $[0, t_f]$, $\mathbf{u}$ denote the known (measurable) inputs of the process, and $\boldsymbol{v}$ is an additive measurement noise vector. The vector $\mathbf{g} \in \boldsymbol{R}^{ng}$ represents the unknown (unmeasured) stochastic time varying input faults of interest, which has to be diagnosed with a FDD algorithm. The function f is assumed to be the first-principles model of a process.

The input faults $\mathbf{g}$ considered in this current work consist of stochastic perturbations superimposed on a specific set of mean values as shown in Fig. 1(a). For example, the inset shows the perturbations around a particular mean value of faults. The input faults $\mathbf{g}$ can be mathematically described as follows:

$$g_i = \bar{g}_i + \Delta g_i \quad (i = 1, \ldots, n_g), \tag{2}$$

where $\{\bar{g}_i\}$ are a set of constant mean values, $\{\Delta g_i\}$ are stochastic variations around each mean value. The statistical distribution of Δg_i is assumed to be time invariant and can be estimated from an offline model calibration algorithm. The constancy of the means $\{\bar{g}_i\}$ can be experimentally inferred from the constancy of measured quantities in Fig. 1(b) such as the manipulated and/or controlled variables while constant input values are used. Fig. 1(b) shows the changes of the measured quantity resulting from the perturbations in input faults.

As shown in Fig. 1(a), the changes in the mean values of $\{\bar{g}_i\}$ follow a Multilevel Pseudo Random Signal (ML-PRS) (Ljung, 1999). The inputs $\mathbf{g}$ described by Eq. (2) are typical in chemical processes that experience both changes in means of operating variables but also additional continuous random perturbations around the means, i.e., the inset in Fig. 1(a). Although, the changes in mean values of inputs for chemical processes are not random since they are often purposely initiated by plant personnel, in this work these changes are assumed to be random to avoid biasing the results towards a particular choice of these changes. In summary, the FDD problem in this work can be defined as follows.

Problem 1 (Fault detection): Detect any stepwise changes in the mean values of $\{\bar{g}_i\}$ in the presence of perturbations. Each mean value will be referred heretofore as to an operating mode.