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Shape anomaly detection for process monitoring of a sequencing batch reactor

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ABSTRACT

Anomaly detection is critical to process modeling, monitoring, and control since successful execution of these engineering tasks depends on access to validated data. Classical methods for data validation are quantitative in nature and require either accurate process knowledge, large representative data sets, or both. In contrast, a small section of the fault diagnosis literature has focused on qualitative data and model representations. The major benefit of such methods is that imprecise but reliable results can be obtained under previously unseen process conditions. This work continues with a line of work focused on qualitative trend analysis which is the qualitative approach to data series analysis. An existing method based on shape-constrained spline function fitting is expanded to deal explicitly with discontinuities and is applied here for the first time for anomaly detection. An experimental test case and a comparison with the principal component analysis method bear out the benefits of the qualitative approach to process monitoring.

1. Introduction

Need for anomaly detection. The advent of increasingly intense data collection strategies for industrial processes suggests that increasing regulatory and efficiency requirements can be met by data-driven methods to model, monitor, and automate engineered process systems. However, data-driven computer-based technologies can only be successful if the data quality produced is guaranteed to be sufficient for automated decision-making and if the optimized process behaves in predictable ways. The data quality of biological processes can be severely deteriorated in many ways, including inadvertent human errors (*e.g.* calibration errors) and naturally occurring phenomena, ranging from events such as the passage of bubbles and particles over long-term processes such as film formation (*e.g.* biofilm growth, deposition, scaling) to sensor aging (*e.g.* corrosion). The processes themselves do not necessarily exhibit normal conditions either. Process faults commonly identified in biological processes include the toxicity effects of inlet streams and changes in microbial community composition or biochemical expression. Successful modeling, monitoring, and automation thus depend on effective tools to detect anomalous data (Nopens et al., 2007; Thomann, 2008; Rieger et al., 2010; Dürrenmatt and Gujer, 2012; Spindler and Vanrolleghem, 2012).

Available methods. A vast literature focuses on the automated detection, isolation, and identification of faults in actuators, processes, and sensors. These techniques are most commonly based on a (quantitative) model which describes data obtained under normal conditions of process operation. An important distinction can be made between techniques using models based on first principles (also known as mechanistic or white-box models, Venkatasubramanian et al., 2003c) and techniques using empirical data-based models (*i.e.* black-box models, Venkatasubramanian et al., 2003b). White-box models are particularly useful when the monitored process is understood to the point of allowing reliable mathematical models of it to be constructed. Black-box models are recommended for cases where the process understanding is limited and large representative data sets are available. Both supervised (*e.g.* classification) and unsupervised methods (*e.g.* clustering, principal component analysis) are popular. Unfortunately, both process understanding and historical data sets are often severely limited, especially for biological processes. Furthermore, extrapolation of the model in time can be challenging due to incipient changes and stochastic variations in the monitored process. Traditional methods for fault detection are seldom applicable without the need for substantial efforts to collect data and/or model the monitored process.

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The promise of qualitative methods. A smaller section of the literature presents qualitative methods as a valuable set of alternatives to the above-mentioned set of methods (Venkatasubramanian et al., 2003a). These methods are based on abstract, coarse-grained representations of data series and process dynamics. White-box models, such as qualitative differential equations (Kuipers, 1994) or signed directed graphs (Maurya et al., 2003), can again be identified. These are used to represent process dynamics qualitatively by focusing on the signs of process states and/or one or more of their rates of change, rather than their exact values. This deliberate lack of precision in the resulting model predictions leads to a high reliability of the resulting predictions even when extrapolated far from the conditions under which the model was identified. However, detailed process understanding is still a requirement since the qualitative models have so far been obtained only by abstracting from a quantitative dynamic model describing normal operating conditions, which is assumed to be available. Qualitative trend analysis (QTA) methods constitute the black-box equivalent (Maurya et al., 2007). In this case, data series of continuous variable measurements are represented by means of episodes, which characterize segments of the series in terms of the signs of one or more derivatives (Maurya et al., 2007). Such abstraction can facilitate the recognition of historical data patterns despite unpredictable variations in the exact data values. Most of the available methods are unsupervised in nature, *i.e.* without specification of the expected patterns. Due to the relatively recent emergence of this field, QTA methods are mostly based on an intuitive recombination of existing quantitative techniques (*e.g.* Dash et al., 2004; Villez, 2015).

Current limitations of qualitative methods. Villez et al. (2013) proposed a formal globally optimal deterministic optimization approach to QTA by recasting the pattern recognition problem as the maximum likelihood fitting of a shape-constrained splines (SCS) function. Solving this problem to a globally optimal level comes at large computational cost. For this reason, a faster and approximate method called qualitative path estimation (QPE) is developed by Villez (2015), offering similar performance at minimal computational cost. Both SCS and QPE methods are currently limited as *(i)* the qualitative patterns which ought to be recognized need to be specified before execution of the algorithm, *(ii)* the analysis is limited to univariate data series, and *(iii)* discontinuous trends cannot be accounted for in a systematic manner. To the authors' knowledge, it is impossible to modify the QPE method to remove this last limitation (see Villez, 2015). In this work, therefore, the existing SCS method is modified to support QTA in the presence of discontinuous trends.

This study. In addition to the modifications of the SCS method, this article also describes for the first time how the SCS method provides a lack-of-fit statistic which can be used for fault detection. The analogy of this approach to the use of the Q or squared prediction error (SPE) statistic commonly used in fault detection based on principal component analysis (PCA, Jackson and Mudholkar, 1979; Kresta et al., 1991) is demonstrated below. Furthermore, this work compares the anomaly detection performances of both SCS and PCA. This article continues with *Materials and methods*, in which the applied data models, anomaly detection methods, and the proposed performance evaluation are initially explained, followed by a description of the analyzed data and their purpose in this study. In the *Results* section, all the results obtained are discussed in detail while the *Discussion* section provides an in-depth analysis. This study is summarized in the last section, namely *Conclusions*.

2. Materials and methods

The modified SCS method and PCA as applied here are described first. This is followed by a description of the studied data sets. An overview of the acronyms and typographical conventions used as well as a list of symbols are given in Appendix A (Tables A.1–A.3).

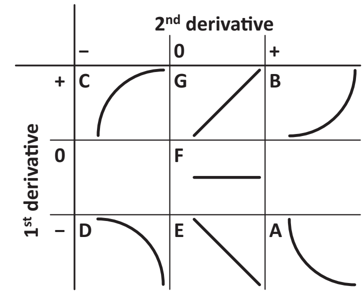

Fig. 1. Primitives. The above scheme includes all triangular primitives defined on the basis of the sign of the 1st and/or the 2nd derivative.

2.1. Methods

Two methods are used for anomaly detection. The first one is a modification of the existing SCS method, while the second one is based on PCA. Both methods result in the computation of a lack-of-fit statistic, namely a sum of squared residuals (SSR). In both cases, this statistic is used to detect anomalous data as explained at the end of this subsection.

2.1.1. Shape-constrained splines

Shape-constrained function fitting is applied here as a way of detecting significant deviations between the shape of a data series and a predefined shape reflecting normal conditions. The following paragraphs show how this problem can be formulated mathematically and solved numerically.

Definitions and notation. In analogy to previous work, the following definitions are used here:

Episode. An episode is an argument interval over which the signs of a function or data series and/or a selection of their derivatives do not change. It is defined by a primitive, a start time, and an end time.

Primitive. A primitive is a unique combination of signs for a value of a function and/or one or more of its derivatives. Each primitive is usually referred to by means of an arbitrarily chosen character. The sign of the first and second derivatives of a cubic spline function are of interest in this work. The primitives are called triangular primitives when the signs for both the first and second derivative are specified (Cheung and Stephanopoulos, 1990). The correspondence between the signs of the derivatives and the characters is given in Fig. 1 and is the same as in Villez et al. (2013).

Qualitative sequence. A qualitative sequence (QS) is a series of primitives. Such a QS is used to describe the assessed or expected shape of a function or data series. A QS does not include the argument locations (transitions) at which a change in primitive is expected or observed.

Qualitative representation. A qualitative representation (QR) is a complete description of the expected or observed shape of a function or time series and consists of a QS and values for the argument values of the corresponding transitions.

Transition. A transition is defined as the argument location where one primitive changes to the next.

Any QS is defined mathematically by means of integers, $s_{e,j}$ ($s_{e,j} \in \{-1, 0, +1\}$), with e indicating the index of the primitive in the QS ($e \in \{1, 2, \ldots, n_e\}$) and j indicating the considered derivative ($j \geq 0$). An unknown or unspecified sign is symbolized with a question mark (?), similar to previous work (Villez et al., 2013). In all cases studied in this work, only triangular primitives are used so that the sign values of the cubic spline function and its third