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Review

Review of adaptation mechanisms for data-driven soft sensors

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ABSTRACT

In this article, we review and discuss algorithms for adaptive data-driven soft sensing. In order to be able to provide a comprehensive overview of the adaptation techniques, adaptive soft sensing methods are reviewed from the perspective of machine learning theory for adaptive learning systems. In particular, the concept drift theory is exploited to classify the algorithms into three different types, which are: (i) moving windows techniques; (ii) recursive adaptation techniques; and (iii) ensemble-based methods. The most significant algorithms are described in some detail and critically reviewed in this work. We also provide a comprehensive list of publications where adaptive soft sensors were proposed and applied to practical problems. Furthermore in order to enable the comparison of different methods to standard soft sensor applications, a list of publicly available data sets for the development of data-driven soft sensors is presented.

Contents

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1. Introduction

Data-driven soft sensors have been developed and implemented for a long time (Fortuna, 2007; Kadlec, Gabrys, & Strandt, 2009). They gained on popularity with the increasing availability of recorded data in the process industries and availability of computational power to process the data. The collected data, also referred to as *historical data*, can be exploited by statistical and machine learning techniques to obtain additional information that can be used to make decisions towards more efficient and safe process operation. This kind of information can, for instance, be an instant prediction of the variables that are related to the product quality, which can be achieved using *o* nline prediction soft sensors (Fortuna, 2007; Gonzalez, 1999; Kadlec et al., 2009), or the estimation of current process state, which can be achieved using *process monitoring and fault detection* soft sensors (Kourti, 2002; Venkatasubramanian, Rengaswamy, Kavuri, & Yin, 2003b; Venkatasubramanian, Rengaswamy, Yin, & Kavuri, 2003c; Venkatasubramanian, Rengaswamy, & Kavuri, 2003a). However, this task is not trivial because historical data are often data rich but information poor (Dong & McAvoy, 1996) and therefore the model building on its basis is a challenging task.

The first generation of data-driven soft sensors relied on offline modelling using the recorded historical data. In such a case, the collected historical recordings are used for the model identification. This step may for instance include the identification of optimal weights of an Artificial Neural Network (ANN) (see e.g. Yang & Chai, 1997) or principal components of a Principal Component Analysis (PCA)-based soft sensor (see e.g. Wold, Geladi, Esbensen, & Ohman, 1987). However, in order to guarantee the success of the offline soft sensors, there are several conditions that have to be fulfilled. Most critically, the historical data has to contain all possible future states and conditions of the process. This includes not only the states in which the process can be operated but also states related to environmental changes, changes of the process input materials, etc. Even if the collected historical data contains all the required process states, another difficulty is to select a model type, and its parameters, in such a way that the model can comprehend all the different conditions. This results in high model complexity, which in turn demands and a large number of historical data for the model development. Additionally, most of the processes are exhibiting some kind of time-varying behaviour and thus require a strategy for online adaptation (Gallagher, Wise, Butler, White, & Barna, 1997). The most common causes for such a behaviour are:

- changes of process input (raw) materials;
- process fouling;
- abrasion of mechanic components;
- catalyst activity changes;
- production of different product quality grades;
- changes in external environment (e.g. weather, seasons).

Especially the last point from the above list is very difficult to estimate during the model design phase and therefore for processes sensitive to the external environment adaptive soft sensing techniques should be used.

As a result of these facts, it can often be observed that the performance of static models starts to deteriorate during their online operation (Kadlec et al., 2009).

The above issues, were identified already in the mid-1990's and first works on the next generation of data-driven soft sensors started to appear (see e.g. Wold, 1993 for one of the first publications on adaptive soft sensing).

To be able to cope with the effects listed above, adaptive soft sensors rely on various techniques for their online adaptation. The first adaptive soft sensors were based on the moving window techniques and recursive updates of the Least Squares (LS), Principal Component Analysis (PCA) and Partial Least Squares (PLS) methods (see Dayal & MacGregor, 1997b; Qin, 1998; Wold, 1993 for some early examples of these methods). Another difficulty of the operation of adaptive soft sensors is that the model has to be steadily supplied with a feedback about its performance as shown in Fig. 1. In such an environment, the soft sensor is first developed using some data pre-processing and predictive techniques selected from a repository of available methods (e.g. LS, ANN, and PLS). The selected techniques are, together with the available expert process knowledge, applied to the historical data and as result a soft sensor is obtained. During the operational, or online, phase the soft sensor is adapted using a maintenance mechanism which relies on: (i) online data; (ii) expert knowledge; and (iii) feedback about its performance.

Furthermore, equipping a soft sensor with adaptive capability requires two tasks to be performed. In the first instance, the need for adaptation has to be recognised by monitoring the performance of the model. This can be achieved by comparing the model output with information acquired from the laboratory analysis. In practical scenarios, this step is often ignored and the models are adapted at periodical intervals or constant forgetting factors are implemented as shown later in this work. Once the need for adaptation has been identified, the actual adaptation is to be performed.

In the case when data pre-processing is applied to deal with data issues like outliers, missing values, etc., the model adaptation has also to include the adaptation of the pre-processing methods. Furthermore, dealing with these issues has to be extended beyond the development phase in order to ensure (during the online phase) that the models are adapted with useful data only, and thus to