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Process Monitoring in Chemical Industries – A Hidden Markov Model Approach

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Abstract

The detection of abnormal events in advance is still a challenge in chemical industries. The earlier it is done, the greater the possibility of at least mitigating losses. This study investigates the performance of a signal processing tool so-called hidden Markov model (HMM) in accomplishing detection tasks. The case study is based on a chemical recovery boiler that belongs to a Kraft pulping mill in Brazil. The identified model, characteristic of normal operating conditions, was exposed to usual situations, namely multiple normal operating states, transient periods, and abnormal events. The detection system was able to reach both mandatory requirements, i.e. early identification of abnormal situations and minimization of false alarm rates.

Keywords: Fault detection, Signal processing tool, Hidden Markov models, Industrial data analysis

1. Introduction

Process monitoring tasks in chemical industries aim to guarantee operating, economic, safety and/or environmental goals. Abnormal situations may result in several losses such as lower production, higher level of emissions, and equipment and personnel damages. This activity has three major tasks: detection, diagnosis, and process recovery to a normal or safety condition [1]. Since faults are in general incipient, deviations from normal operating conditions are smaller at the beginning; consequently, reaching early detection without the support of a computer-based system is practically unfeasible. Besides early detection, another challenge in process monitoring is the spatial overlapping problem among distinct fault classes. Therefore, once some events may only be distinguished from each other by taking into account their order of occurrence, it is worthy to consider a time series modelling. Most of the applications are normally based on residue metrics, and another way to approach the fault detection and diagnosis matter is using signal processing tools [2]. Thus, the so-called hidden Markov model (HMM) method appears as a promising decision support system for helping control room operators to accomplish process monitoring tasks. This data-driven technique belongs to the signal processing field and constitutes an alternative approach for the development of Fault Detection and Isolation (FDI) systems. This work investigates the performance of the hidden Markov model (HMM) technique in accomplishing detection tasks of abnormal situations in industrial chemical processes. The case study is based on a chemical recovery boiler that belongs to a Kraft pulping mill located in Brazil. Ref. [3] contains a review about the fault detection and diagnosis subject. Studies concerning process monitoring activities using HMMs on computer-simulated cases are those by [4-9].

2. Hidden Markov model (HMM)

Every chemical process is under random influences due to an inherent variability present in, e.g. raw material, air temperature, and stream compositions. Thus, measurements of process variables may be seen as realizations of an underlying stochastic process. Thus, normal operating conditions may be described by particular probability distributions, which fail in case of changes in process conditions [3]. (It means a change in mean and/or standard deviation in case of using Gaussians.) This is the motivation for putting together the signal processing tool so-called hidden Markov model (HMM) and the chemical process monitoring activity, once it is capable of identifying changes of statistical nature in signals (composed by measurements of process variables) over time. The successful applications are in the speech processing field, including both speech recognition and speaker verification, since the seventies [10].

2.1. Fault Detection Tasks with HMMs

The goal of the hidden Markov model technique is to model sequential data. Fig. 1 shows the input-output relation for them, in which the input is a temporal sequence of T vectors ($O = \{o_1,o_2,\ldots,o_T\}$), and the output is a likelihood value ($-log[P(O|\lambda)]$), which is a measure of the capacity of the model (λ) in generating the observed data (O). The logarithmic form is preferable in order to avoid underflow computational problems. After the occurrence of an incipient fault, likelihood values from an HMM representing normal operating conditions are lower over time due to changes in the underlying distribution. Thus, the method can be defined as a sequential pattern recognition tool. The temporal sequence (or pattern) is a set of symbols (discrete case) or real vectors of same size (continuous case). Such elements (o_t) are called frames and each one carries a piece of information about the system at a given time t [10].

$$O=\{o_1,o_2,\ldots,o_T\}) \longrightarrow \boxed{\text{HMM } (\lambda)} \longrightarrow -log[P(O|\lambda)]$$

Fig. 1. Input-output relation for HMMs, where O is the observation sequence (O) and ($-log[P(O|\lambda)]$) is the likelihood function.

2.2. Mathematical Formulation

Hidden Markov models are a doubly stochastic process, in which the former is responsible for the state-transitions ($P(q_t|q_{t-1})$), whereas the latter is related to the observation-emissions ($P(o_t|q_t)$). As the state-transitions rule follows the Markov property, i.e. q_t depends only on q_{t-1}, the HMM concept is an extension of Markov chains. The difference between both classes of models relates to the second process since in Markov models the relationship between states and observations is deterministic. The *hidden* term in HMMs is due to the fact that the underlying Markov chain is not directly observable. Table 1 shows the three parameters to specify discrete HMMs, where M_D is the number of distinct observation symbols in the emission probability distributions (one for state), and N is the size of the discrete state space. A compact notation for these parameters is given by λ, i.e. $\lambda = (\pi,A,B)$. For the continuous case (used in this work), the B matrix is replaced by probability density functions, whose usual representation is a finite mixture of Gaussians, as in Eq. (1), where o_t is the observation vector at time t, M_C is the number of mixture components per state, and c_{jk} is the mixture component (subjected to stochastic constraints), μ_{jk} is the mean vector, and Σ_{jk} is the covariance matrix, for the kth mixture component in the state j. The parameters π and A are the same as in the discrete case [10].

Table 1. Elements of discrete HMMs.

Parameter	Description	Formulation
$\boldsymbol{A}=\{a_{ij}\}$	State-transition probability distribution	$a_{ij}=P(q_{t+1}=j \mid q_t=i)\,,\ 1\le i,j\le N$
$\boldsymbol{B}=\{b_j(k)\}$	Emission probability distribution	$b_j(k)=P(\boldsymbol{o}_1=v_k \mid q_t=j)\,,$ $1\le k\le M_D\,,\ 1\le j\le N$
$\boldsymbol{\pi}=\{\pi_i\}$	Initial state probability distribution	$\boldsymbol{\pi}_i=P(q_1=i)\,,\ 1\le j\le N$

$$b_j(\boldsymbol{o}_t)=\sum_{k=1}^{M_C} c_{jk} N(\boldsymbol{o}_t,\boldsymbol{\mu}_{jk},\boldsymbol{\Sigma}_{jk})\,,\ 1\le j\le N \tag{1}$$

3. Case study

The case study is based on a chemical recovery boiler from a Kraft pulping mill in Brazil. One of its goals is to produce high pressure steam for electric power generation as well as heat transfer operations. The fuel is the residual liquor originating from the cooking stage of wood chips. The equipment has two regions: a furnace, where the combustion of the liquor and the recovery of specific inorganic compounds occur, and a convective heat transfer section, as in power boilers, co-responsible for transforming fresh water in high pressure steam. For that, this region has a series of heat exchangers, namely super-heater, boiler bank, and economizer, as shown in Fig. 2. A risk situation of great concern during boilers' operation refers to water leaks in tubes of the heat exchangers due to the possibility of the water-smelt contact. The smelt is a pool of melting sodium-based compounds over the furnace floor, with a surface temperature of about 850 ^{o}C, which is more than enough to cause an explosion in case of contact with water [12]. These leaks are mostly caused by weld failures, and corrosion, fatigue and erosion of tubes [13]. Common mill practices are still based on operator's actions, through patrols around the boiler and the monitoring of key variables mainly the fuel gas temperature along the section [14]. Thus, in a specific way, this study investigates the potential of the hidden Markov model technique in detecting abnormal events in the heat transfer section of the boiler under analysis, which may lead to risk situations, e.g. water-smelt contact. The considered region is enclosed by the super-heater and the boiler bank, and the monitored variable is the fuel gas temperature.

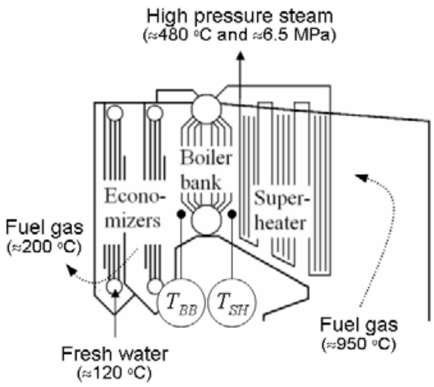


Fig. 2. Sensors position for measuring the fuel gas temperature after both heat exchangers the super-heater and the boiler bank: T_{SH} and T_{BB}, respectively.

3.1. Data Set

The data set comprehends one month of operation, with a sampling interval of five minutes. Table 2 presents the collected variables, where F_{BL}, which determines the operating states in the boiler, may be considered discrete for this particular mill. Fig. 2 shows the position of both temperature sensors in the convective heat transfer section. Other variables were collected in order to verify the operating conditions along this period.

Table 2. Variables collected in the chemical recovery boiler.

Operating Variable	Code	Range	Unit
Black liquor flow rate	F_{BL}	14-53	m^3/h
Fuel gas temperature after the super-heater	T_{SH}	453.8-771.1	^oC
Fuel gas temperature after the boiler bank	T_{BB}	282.0-397.8	^oC

4. Methodology

4.1. Model Identification Step

The goal is to identify a representative HMM for the boiler under normal operating conditions. A continuous HMM is used in this work, and each observation sequence is composed of 5 real vectors, i.e. $O = \{o_1, o_2, \ldots, o_{T=5}\}$, where $o_t = [T_{SH}\ T_{BB}]_t'$. The definition of the number of vector so-called frames should take into account the system dynamics, being smaller in case it is faster, and bigger, otherwise. As measurements are available each 5 minutes, a sequence is completely full after every 25 minutes. The data was divided into three subsets: training and validation (used in this step), and test. Initially, plenty of models are generated by varying the number of mixture components per state (M_C), from 1 up to 3, and the number of states (N), from 2 up to 22. The topology of the models is a fixed parameter being used the ergodic one, in which there are no restrictions regarding state-transitions (A matrix), and the covariance matrix (Σ) is constrained to be diagonal in order to reduce computational efforts. Model selection is based on the likelihood function being selected the one that gives the highest mean value calculated onto the validation subset. The Baum-Welch algorithm, based on the Maximum Likelihood Estimation (MLE) principle, is employed in this step [15]. Finally, an upper control limit ($UCL = \bar{x} + 3 \cdot s$) for defining a normal operating window is calculated, where $\bar{x}$ and s are the mean and the standard deviation of the likelihood function, respectively, considering the training and the validation data.

4.2. Testing Step

A reliable monitoring system has two requirements: early detection of abnormal events, and simultaneously minimization of false alarm rates. This step aims at exploring both issues related to detection tasks. For that, the model selected before is exposed to three usual scenarios during the operation of the equipment: (a) unseen normal operating states, which is given by the black liquor flow rate (F_{BL}), (b) mixed observation sequences, composed of temperature measurements collected during normal transient periods, which is a result of a change in the liquor flow rate, and (c) abnormal situations. There is none register of such kind of event in the database, according to daily mill reports, and hence a real one was simulated. As the boiler operates in a continuous way, a trend plot for the likelihood function (the model output) arises over time, which constitutes a source of information about the operating condition of the equipment. The Forward algorithm is used to calculate the model output [10].

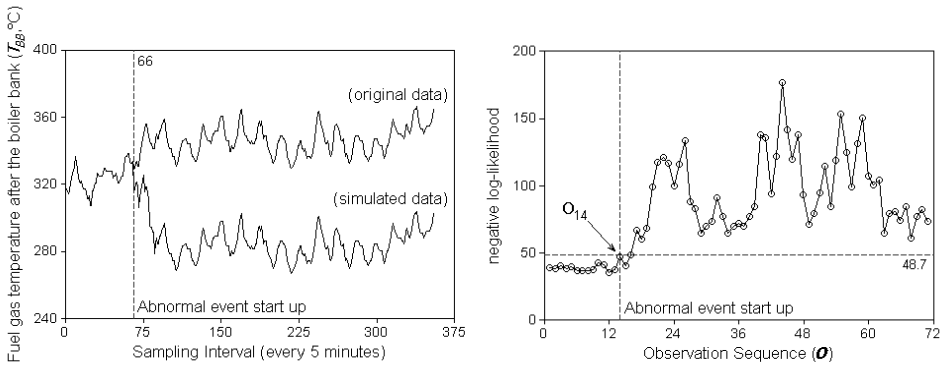
5. Results and Discussion

5.1. HMM Identification

The training, validation, and test subsets contain, respectively, 687 (≈ 49%), 342 (≈ 24%), and 369, observation sequences. A cleaning procedure was carried out before such division. Test data correspond to the last week in the monthly database. The selected HMM, characteristic of normal operations, among the 63 candidate models, is the one with 2 mixture components per state (M_C) and 20 states (N). The upper control limit (UCL) is equal to 48.7. A tendency of having likelihood values beyond it acts as a warning about the possibility of an abnormal event in the region enveloped by the super-heater and the boiler bank in the convective heat transfer section of the boiler.

5.2. Testing step

The goal of this step is to get the behavior of the HMM previously identified when subjected to usual situations during the operation of chemical recovery boilers. In relation to the first two scenarios: unseen normal operating conditions and mixed observation sequences, the model was able to deal with both of them, once the associated likelihood values fell inside the normal operating window (i.e. below the upper limit control). This is a desirable characteristic regarding the matter of minimization of false alarm rates, since such conditions are associated to normal operations. Last scenario concerns the first step in monitoring activities, i.e. the detection task. Due to the lack of abnormal events in the database, according to daily mill reports, a possible one in a practical point of view was simulated. A decrease in the fuel gas temperature after the boiler bank (T_{BB}) was introduced in the real data, at a fixed rate of 1 ^{o}C/min, as shown in Fig. 3(a). It may be caused by water leaks in boiler bank tubes, an incident that represents a potential risk of explosion due to the possibility of the contact between the water and the pool of melting chemical compounds over the furnace floor. Fig. 3(b) shows the resulting likelihood plot. The first thirteenth observation sequences (O_1,O_2,…,O_{13}) refer to a normal condition, and the abnormal event starts at O_{14}. The model is able to detect it in their initial stage, and as times goes by, output values are higher and higher once the probability of the model in generating the sequences diminishes. This model behavior can be explained by the change in the relationship between T_{SH} (the fuel gas temperature after the super-heater) and T_{BB}, which is an absent characteristic in both prior scenarios.



(a) (b)

Fig. 3. (a) Simulation of an abnormal situation in the fuel gas temperature after the boiler bank (T_{BB}), by the introduction of a decreasing at a fixed rate of 1 ^{o}C/min, and (b) resulting likelihood plot when the HMM characteristic of normal operating conditions is subjected to this event.

6. Conclusions

A HMM, representative of normal operating conditions, was subjected to three scenarios of great interesting for chemical industries concerning the management of abnormal situations, namely unseen normal operating states, mixed observation sequences, and abnormal events. The results are promising with regard to both aspects early detection and minimization of false alarm rates, which are requirements for obtaining reliable detection systems. The resulting trend plot for the likelihood function is valuable source of information since it is capable of providing the current state of the process and then its tendency, by making associations between states of the Markov chain and operating states of the process, and of warning about the possibility of coming deviations from the normal condition. In case of considering multiple abnormal situations the magnitude of the model output (i.e. the likelihood value) may be used for the discrimination (or at least the identification of a subset) of them. In brief, chemical process monitoring activities may take advantage of decision support systems based on hidden Markov models.

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