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Assessment of two qualitative trend analysis tools for process control

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Abstract:

In wastewater, sensors are often prone to drift. Nevertheless, their signals still contain valuable information such as their first and second derivative. In this study, two algorithms to extract the signs of the signal's derivatives are tested on a UV-Vis based nitrite estimation signal. The algorithms fit a given sequence of shapes onto the signal and identify the location of the resulting qualitative features (QF) (i.e., minimum, maximum, inflection points). Both algorithms were first developed for offline batch analysis and are now tested in as an online tool. Our initial results suggest that SCS and QPE perform relatively similarly well for the given data set.

Keywords: qualitative trend analysis, nitrite, UV-Vis, urine nitrification, stabilizing control

Introduction

Wastewater collection and treatment systems are harsh environments for sensors. Thus, sensor faults such as drift or shift are common phenomena. For fast-changing faults such as shifts or outliers, a wide range of fault-detection methods exist (e.g., Venkatasubramanian et al., 2003). However, detecting slowly and gradually changing faults, such as drift, often requires redundant information. Therefore, we hypothesize that for these cases we can avoid the complex fault detection step by using other methods to extract automatically the relevant information from drifting sensor signals.

An example of such slow-drifting sensor is a UV-Vis based soft-sensor for nitrite (Thürlimann et al., 2016) in a source separated urine nitrification (UN) reactor (Fumasoli et al., 2016). Its sensitivity is relatively constant but the sensor drifts making the absolute value not trustworthy. However, keeping nitrite concentrations in a narrow concentration range (<5-10 mgN/L) is essential for process stability. In a previous modeling study (Thürlimann et al., 2017), an alternative nitrite controller was presented that takes advantage of the stable sensitivity but neglects the absolute value of the soft-sensor estimation. At the same time, the controller induces nitrite oscillations in the reactor to generate an information rich nitrite signal by increasing and decreasing the pH setpoint and in turn the feed rate. This feed rate changes will induce net nitrite accumulations and degradation, respectively. The inflection point in the decreasing signal is the most informative point. It indicates the end of the substrate induced NOB-inhibiting conditions and the onset of the substrate-limiting condition. Despite the added noise and drift on the simulated nitrite signal, the Qualitative Path Estimation (QPE) algorithm (Villez, 2015) successfully located the inflection points and allowed for a safe and efficient operation in a simulation environment.

In this study, we intend to go one step further and test the previously used QPE and another qualitative trend analysis method (see below) on a real-world UV-Vis soft-sensed nitrite signal. The real world signal exhibits significant differences to the modelling exercise: Partly because the simplification in the model leads to smoother nitrite dynamics as in a real reactor and partly because the sensor induced noise and drift was modeled as a Brownian motion. In contrast, the noise and drift in the real signal is most likely less random and may be harder to filter out. The methods tested are the QPE as in Thürlimann et al., (2017) plus the Shape Constrained Splines methods (SCS) (Villez and Habermacher, 2016). To broaden the scope even further not only the downward inflection point (DIP) but also the other three qualitative features (QF) minimum (MIN), maximum (MAX) and upward inflection points (UIP) will be considered.

Both algorithms were developed originally for offline batch diagnosis and differ regarding speed and optimality. We hypothesize that the SCS method will perform better in the real-world environment as it should be less prone to noise and requires less tuning.

Methods

Reactor and operation: The underlying nitrite data was obtained in a UN reactor. The nitrification is alkalinity limited. Thus, only 50% of the ammonia is oxidized (Fumasoli et al., 2016). Every minute the UV-Vis spectrum was recorded by a 2 mm path length spectrolyser (S::CAN, Austria).

PC and human based feature identification: Both algorithms fit a predefined sequence of primitives (i.e., episodes in which the sign of the first and second derivative are constant) to a given data series. The switches between the episodes are the locations of the QF and are named *transitions*. In the presented case, the four following features MIN, UIP, MAX and DIP have to be identified. The QPE is working with a moving window approach to filter the signal and to extract probabilities for the signs of the derivatives. A Viterbi algorithm is used to match the quantitative information with the primitive. The SCS in contrast places a specified number of knots along the time series at which the spline functions are fixed. With a branch-and-bound algorithm, the locations of the transitions are optimized. Both methods were developed for offline batch analysis. One has to trade off optimality, which is best with the SCS method, against computational efficiency, which is best with the QPE method. After every 18^{th} measurement, the whole data set is analyzed and the primitives are fitted on the signal. The knot distance of the SCS is 180 samples; the filter length of the QPE is four times the knot distance (i.e., length of the support windows of the spline basis functions). Furthermore, three independent people were given the raw signal printed and were asked to identify the same transitions as the algorithms. These locations should indicate if there is a human based ground truth about the locations of the QF.

Results

Feature identification: Figure 1 illustrates the location of the four QF in the final analysis with the whole nitrite time series (dashed line: QPE, full line: SCS and full line with circles: three independent human visual judgments). The results show that in a posteriori offline batch analysis the algorithms do not identify the same locations for the QF nor do they always agree with the human judgments. The MIN is apparently easy to identify with the human eye, but not so for the algorithms. A remarkable alikeness of all five identifications is shown for the UIP. The DIP and the MAX show a near-perfect agreement between the algorithms but no agreement with the human judgments.

Figure 2 illustrates the test results in view of online application - as needed for automated control. The location of the four QF are plotted as a function of the number of data points included in the analysis (i.e., time). This reflects the online performance of the algorithms. The 1:1 line indicates the earliest possible placement of a feature onto it (i.e., the first time the point is included in the analysis). The comparison reveals that QPE apparently performs better in terms of stability of the solutions once they are found. This means that it's less sensitive to new data points added which makes it easier to judge if a solution is stable, and therefore acceptable. However, it takes the QPE more data points to reach an acceptable level of agreement (e.g. DIP around 1700 vs. around 1500 for SCS).

Conclusion & Outlook

The qualitative trend analysis methods QPE and SCS perform similarly well when used as an online tool. Not only drifting signals such as the presented turn out to be useful when processed with these algorithms but also relative measurement such as redox potential could potentially be more useful.

In terms of the intended nitrite controller a further key indicator of the analysis will be incorporated in the controller. Given that multiple series of primitives are fitted onto the signal, the ranking of the resulting

RMSR may allow locating the transitions within a shorter period of time. At the time of writing such a solution is implemented on a pilot scale reactor and results will be presented in the anticipated conference paper.

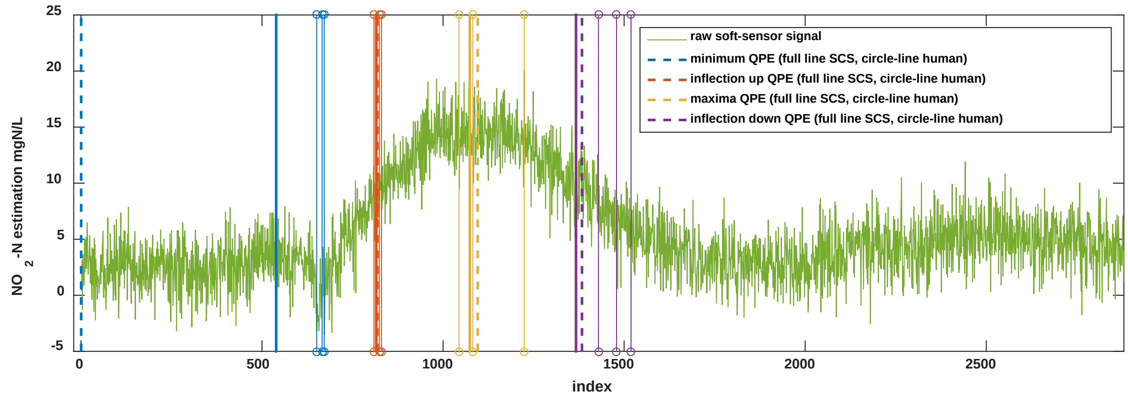

Figure 1 Nitrite estimation time series and location of qualitative features given the whole data set. Full lines: Shape constrained splines results. Dashed lines: Qualitative Path Estimation results. Full line with circles: Three times independent human judgment.

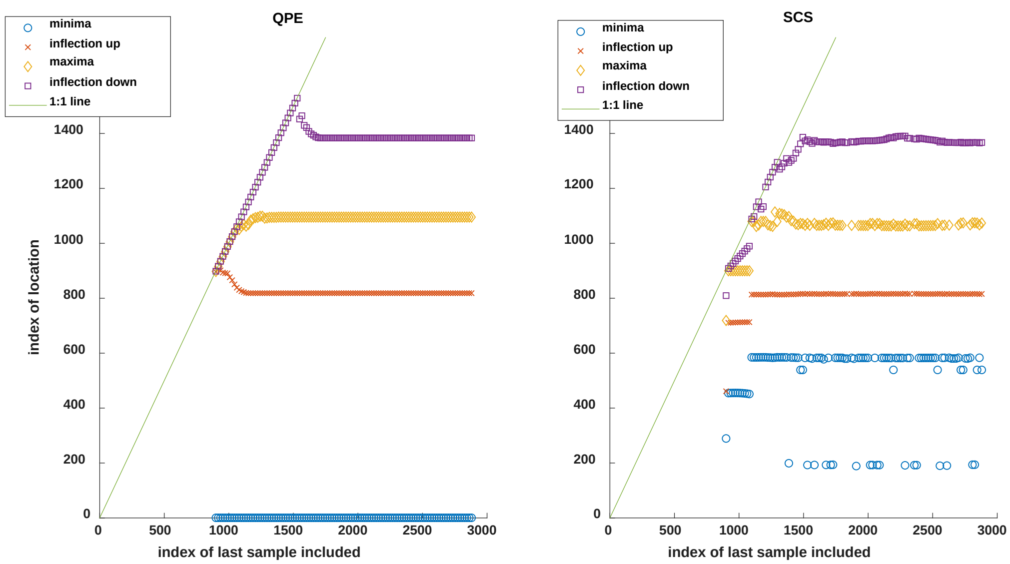

Figure 2 Index of locations of qualitative features as a function of the index of the last sample included in the analysis.

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