

Measuring Cause and Effect between Process Variables

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Abstract

Disturbances in chemical processes spreading through plants affect a number of process variables. The operator or the monitoring scheme in place often detects the disturbance at a variable critical to the process. This variable might not be close to the actual cause and isolation of the root cause becomes therefore a task for the control engineer. The aim of this study is to find ways of identifying cause and effect and thus the direction of propagation of a disturbance using only historical data of the process variables. A recently introduced method, predictability improvement (PredI), is based on embedded vectors and finding their nearest neighbors. The modified PredI algorithm works by exploiting, firstly, time delays which often occur between two measuring points and, secondly, attenuation of the signature of the disturbance related to the distance of the root cause. A new case study of an industrial reaction process is presented. The modified PredI method is applied to a disturbance observed by the operators at the bottom of the reactor and successfully shows that the disturbance originates from a root cause further upstream.

1. Introduction

Fault detection schemes involve the close observation of process variables and control loops. A number of indices have been established to measure the increased variability of variables and loops [1], [2]. An alarm is raised if a variable or calculated index exceeds a predefined threshold. However, this might not be the variable that actually caused the disturbance. Isolating and diagnosing the fault is therefore an important and often challenging task.

Propagation paths in case of normal operation and disturbances have been previously investigated with statistical methods based on probability density function. Chiang and Braatz [3] used the Kullback-Leibler information distance to identify broken relationships when a fault is present. A requirement for the identification,

however, is the existence of a causal map that has to be derived from expert knowledge. The concept of transfer entropy [4] can measure dependencies without constructing a model. The propagation path of the disturbances can be retraced and the root cause isolated. One of the shortcomings of these approaches is that the estimation of the probability density function requires a large amount of data which is not always available, especially if the disturbance only lasts for a short time.

In this article, the statistical method of nearest neighbors is proposed to measure cause and effect, or directionality, between two process variables with using only a limited number of measurement samples. With the availability of high performance PCs a new class of statistical methods has emerged that rearranges the historical data as embedded vectors and calculates the nearest neighbors of each embedded vector. If the nearest neighbor is identified by the use of a second variable, the method becomes a measure of predictability from the second variable to the first and hence a measure of directionality. Čenyš *et al.* [5] introduced a measure to establish whether two systems are related. Wiesenfeldt *et al.* [6] extended the measure to a single step prediction error to measure bidirectional coupling of two systems through uncertainty. The method used in this article is a modification of the predictability improvement (PredI) by [7]. The PredI algorithm extends the approach by Wiesenfeldt *et al.* to measure the reduction of uncertainty of one variable with additional knowledge of a second variable and has thus a parallel structure to the method of transfer entropy but without the shortcoming of requiring a very large data set.

The cause and effect relationships can be best represented in causal models of the process [8]. Qualitative models in form of digraphs are commonly used and a final result of the cause and effect analysis using the method of transfer entropy or nearest neighbors will be the automated construction of such a model

The article is organized as follows. In Section 2, the directionality measure using the principle of nearest neighbor methods is introduced for analyzing oscillating

disturbances. The algorithm for computing the PREDI measure is given together with guidelines for setting the parameter. In Section 3, graphical representation and construction of digraphs are suggested once the measure has been calculated. The application of the PREDI measure to a case study of a reaction process is given in Section 4.

2. Directionality measure

A persistent fault or disturbance often manifests itself as a combination of a periodic oscillation and statistical noise. The oscillation can originate from a variety of causes including sticking valves, instrumentation failures, tuning problems and process inherent instabilities. The signature of the fault changes as the disturbance travels in the process. This change through the process dynamics can be classified as

- Time delay
- Attenuation

The time delay is caused by the fact that it takes time for the disturbance to propagate along the process flow from one physical measuring point to the next. The time delay of two pure oscillations cannot be measured straight forwardly because a variable occurring before a second variable by 120° could also be lagging by 240° to the second variable. Furthermore, if the time delay is small the sampling interval may be larger than the time delay. Exploring the attenuation of the disturbance is useful in these circumstances. Most processes act as low passes and filter the high frequency components of an oscillation. The disturbance will have a smoother shape the further it is away from the root cause. Linear methods such as cross-correlation can measure the time delay between two nearly identical signals but if the functional distortion is too strong it will give no useful results. The concept of predictability improvement, however, incorporates both time delay and attenuation of the signal to measure the causal relationship.

2.1 Nearest Neighbors

Directionality is measured by comparing the predictability of a future value of a first variable if the past values of a second variable are given against the predictability of the second variable if the past values of the first variable are given. The concept is based on the construction of a state space estimate using the historical data points of the process measurements. For this purpose, embedded vectors are formed for process variables X and Y of length: $\mathbf{x}_i^M = [x_i, x_{i-1}, \dots, x_{i-M+1}]$ and $\mathbf{y}_i^M = [y_i, y_{i-1}, \dots, y_{i-M+1}]$. Here, i is the time index and M the number of time samples or embedding dimension. The number of embedded vectors is $N-M+1$ where N is the length of the

sample sequences X and Y . The corresponding future values, or one-step-ahead-predictions, are defined as x_{i+h} and y_{i+h} . The number of steps predicted in the future h is called the prediction horizon.

Algorithm for determining directionality

Step 1 finds k nearest neighbors $\mathbf{x}_{nm,i}$ of \mathbf{x}_i .

Step 2 compares the corresponding future value of y_{i+h} with future value of the k nearest neighbors $y_{nm,i+h}^j$.

$$p_i(Y|X) = \frac{1}{k} \sum_{j=1}^k \|y_{i+h} - y_{nm,i+h}^j\| \quad (1)$$

Step 3 repeats for all embedded vectors and compute average statistic ($l = N-M+1-h$).

$$p(Y|X) = \frac{1}{l \cdot \sigma_y} \sum_{i=1}^l p_i(Y|X) \quad (2)$$

Step 4 computes with exchanged x and y and compare the two measures.

$$P(X|Y) = p(Y|X) - p(X|Y) \quad (3)$$

Here, σ_y is the variance of time series y . The smaller the error between the future value y_{i+h} and the predicted future value $y_{nm,i+h}$, as calculated in step 2, the better is the prediction of X to Y . Thus, the final prediction measure $P(X|Y)$ in step 4 is the difference between X predicting Y and Y predicting X . The original measure p is asymmetric, $p(X|Y) \neq \pm p(Y|X)$, which allows a statement of directionality. Scaling by variance σ_y in step 3 ensures that the measure lies within a range from zero to approximately one. The measure can be slightly larger or smaller than 1 because the number of nearest neighbors and repetitions, k and $(N-M+1)$, is finite. The computational effort increases with N and M and decreases with h because the distance between all $(N-M+1-h)$ embedded vectors has to be calculated and assessed. The computation of the distance becomes more elaborate if the embedding dimension M is higher. When using vector oriented software for implementation, the computational effort is most affected by the length of the time sequence, N and increases with N^2 .

2.2 Guidelines

Adjustment of the parameters is particularly straight forward if a period of oscillation exists. Constructing embedded vectors gives the basis for a state space model of the process. The parameters specified for the construction of the vectors are crucial for the result of the directionality measures. The parameters are embedding dimension M , the prediction horizon h and the number of samples of the two time sequences. Empirical tests have been carried out for a number of data sets and the guideline parameters in the following have shown to give good results for most applications.

Embedding dimension: $M=4$. The length of the embedded vector equals to the dimension of the estimated state space. If the embedding dimension is set too high, no good predictors can be found for both variables even if one is better than the other. The opposite case is true for a too small dimension. Both variables will be good predictors and no strong differentiation is possible.

Number of samples and sub-sampling: $N=400$. Restrictions for the number of samples are recommended for a number of reasons. If the number is too low then not enough relevant features are captured to draw relevant conclusions. Since the computational effort increases significantly with increasing N the number must have been limited by an upper bound which depends on the computational capacities. Also, the time during which the disturbance arises could be limited. Sub-sampling is recommended if more than 40 samples per cycle are captured.

Prediction horizon: $h=1$. In the definition the prediction horizon was set to h when looking at one-step-ahead-prediction. For the optimal result, the prediction horizon is equal to the actual time lag between the two sequences analyzed. As the delay is usually unknown, setting the prediction horizon to one as suggested by Feldmann and Bhattacharya [7] gives satisfying results if the sequence is not oversampled, that is, all the time dynamics of the process are in the same range as the sampling rate.

A further change in the construction of the embedded vectors can be achieved by including the past values of y in addition to x when predicting y_{i+1} . This is equivalent to a feedback structure in the state space. In addition to the time embedding, the number of nearest neighbors has to be chosen.

Number of nearest neighbors: $k=15$. The number does not influence the result of the nearest neighbor method significantly. The number has to be statistically relevant but too if chosen too large, it makes the result irrelevant.

Because of the generic approach of the method of nearest neighbors the data is not restricted to be of oscillatory nature. However, optimization as discussed above is aligned to the oscillatory case.

3. Graphical representation

The directionality measure established in Equation (3) expresses coupling between two variables x and y . A positive value of $P(X|Y)$ indicates that x influences y , a negative value the opposite case. The measure can be calculated for all combinations of n process variable, i.e. $n(n-1)$ combinations. A way of presenting these directionality measures is a bubble chart. In a bubble chart, the driver variables are listed on the y-axis while the response variables are on the x-axis. At the intersection of

driver and response variable a bubble whose size reflects the value of the directionality measure is placed. Thus, the most important relationships are easy to detect.

As a final result, a graph that allows backward inference for the root cause is desired. Digraphs are graphs with directed arcs between nodes. The nodes represent process variables and the arcs the relationship between the variables, that is, the causality measure. Several arcs can lead from and to a node. When constructing the digraph the number of detected relationships has to be reduced in some cases since duplicated dependencies might occur. As an example, a process variable PV1 might influence a variable PV2 which in turn influences PV3. The causality measure may detect not only these relationships but also a dependency between PV1 and PV3, probably less prominent. This dependency has to be rejected when constructing the digraph.

Most of the time, digraphs are constructed using expert knowledge or a mathematical model in form of differential and algebraic equations of the process. Here, the digraph for fault diagnosis is derived from the historical process data and the causality measure. The consistency to models gained from the process schematic helps to understand the root cause of the disturbance.

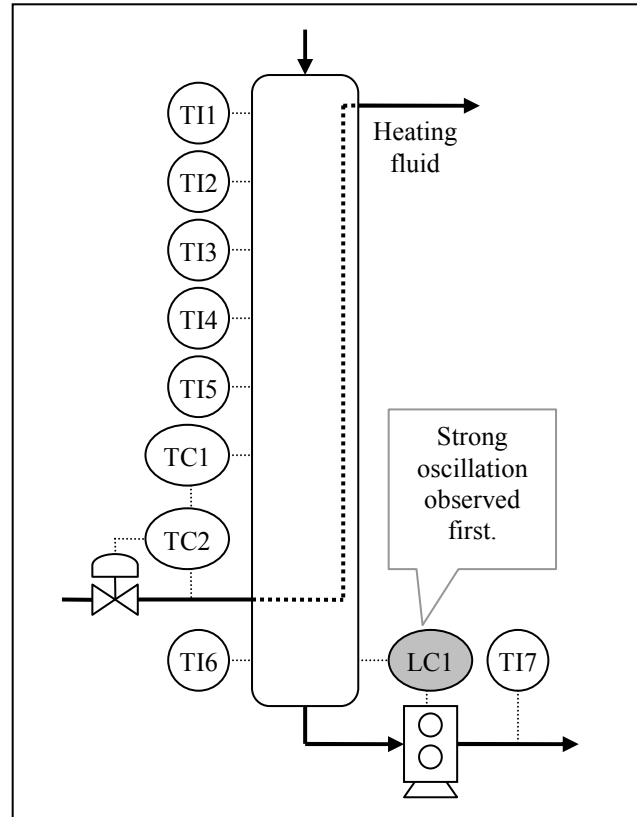


Figure 1. Process schematic of industrial case study.

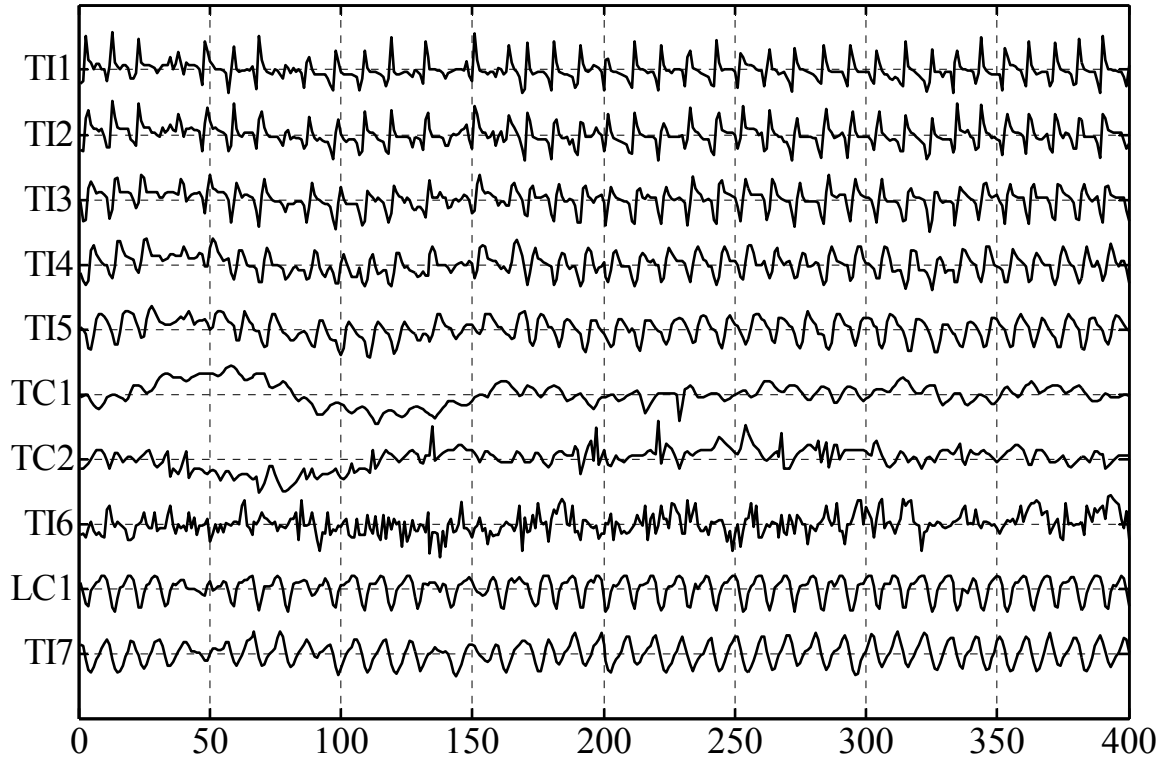


Figure 2. Time trend in samples of process measurements for the industrial case study.

4. Industrial case study

The process schematic of the reaction process is shown in Figure 1. Five temperature measurements are taken in the top section of the reactor above a point where heating fluid is pumped through the tray structure to control the temperature. Controlled temperatures are the inflow of the heating fluid and the temperature right above the inlet which are controlled in cascade. An additional temperature measurement is taken near the outlet of the reactor. The outflow at the

bottom of the reactor is controlled by the level on the bottom tray and a temperature measurement further downstream is available. During operation of the reactor system a strong oscillation was observed by operators at the level at the bottom of the reactor. The level measurement and control is a crucial parameter in the process and closely observed. After the alarm was raised the first reaction was to check whether poor tuning was the root cause. The control engineer also checked all other available reactor process measurements for oscillations of the same period. The time trend of all measurements indicated in the process schematic is shown in Figure 2. Oscillations with the same period as the level affect a number of the temperature measurements along the reactor. All measurements apart from the controlled temperatures TC1 and TC2 as well as the temperature TI6 show strong evidence of the disturbance in the time trend.

The hypothesis posed is that the disturbance is caused further upstream. The task for the directionality measure is to accept or reject the hypothesis.

4.1 Application of directionality measure

An example of the mechanism for the nearest neighbor method can be shown by investigating the relationship between TI4 and TI5. In the top panel of Figure 3 (a) a data point of temperature measurement TI5 is chosen (filled circle). The corresponding embedded vector of temperature TI4 is shown by the filled circles in the lower panel. In a next step, the nearest neighbors of the embedded vector are found which are indicated in the same figure by unfilled circles. The corresponding future values are shown in the upper panel. It can be seen that these are good predictors because the difference to the original sample point, indicated by error bars, is small. In Figure 3 (b) the role of TI4 and TI5 is swapped. The embedded vectors of TI5 now predict future values of TI4. The error bars are larger than for the alternative case so that TI5 can be interpreted as a poor predictor of TI4.

The result for all combinations of process measurements is shown in Figure 4. All values for the directionality measure which are greater than 0.1 are considered and highlighted in grey. Firstly, a group with strong directionalities between the temperature measurements at the top of the column can be observed

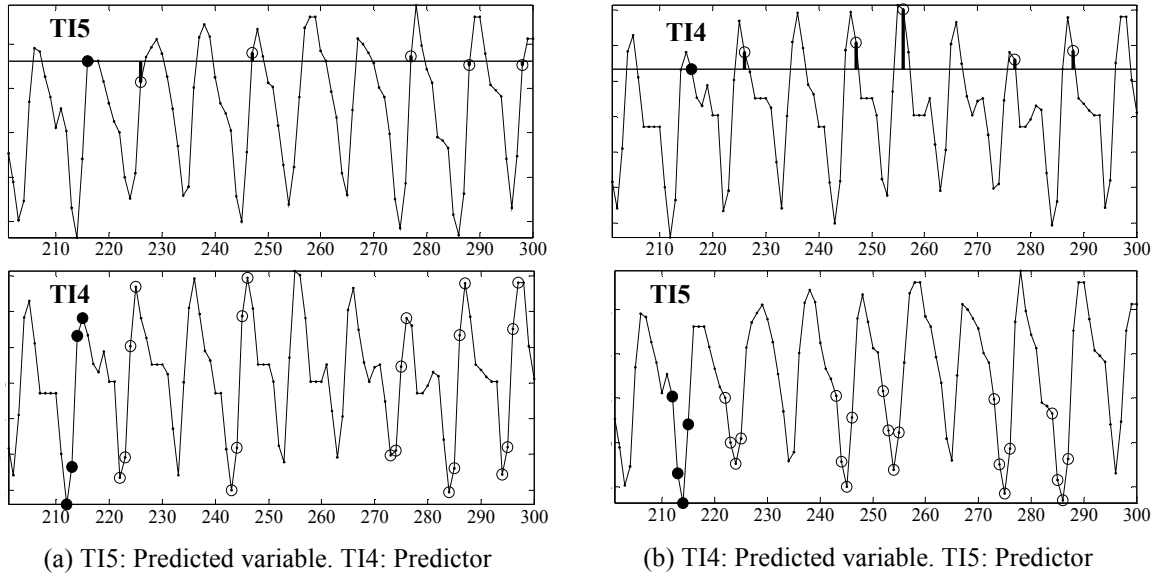


Figure 3. Finding the nearest neighbors: (a) the future values of TI5 (upper panel) predicted by embedded vectors of TI4 (lower panel) are good estimates (small error bars in upper panel); (b) vice versa, TI5 gives a poor estimate for TI4 (large error bars in upper panel)

pointing towards a sequential order from TI1 to TI5. More importantly, the level measurement LC1 is influenced by TI2, TI5 and TC1. However, the other temperatures TI1, TI3 and TI4 do not show this direction. The group of controlled temperatures, TC1, TC2 and TI6 must be viewed separately since the disturbance is not very significantly represented (see Figure 2).

4.2 Construction of digraphs and discussion

The results in the bubble chart in Figure 4 are converted into a digraph as shown in Figure 5 (a). There are no dependencies to TI6 which shows a noisy behavior, see Figure 2. It is believed that the output of sensor TI6 was not strongly related to the actual process temperature, due to sensor installation issues.

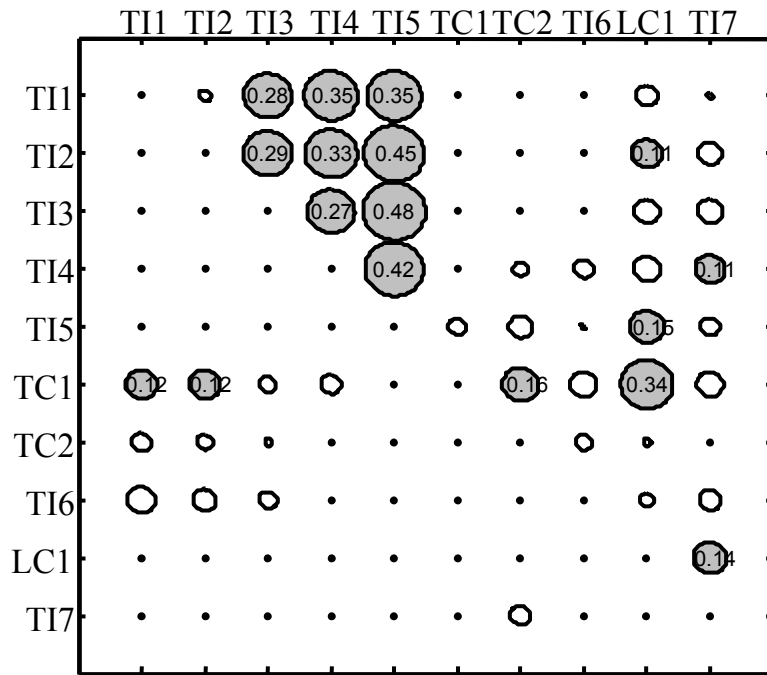


Figure 4. Overview of all directionality measures in a bubble chart. Variables on the vertical axis influence variables on the horizontal axis by the value indicated in the intersecting bubbles.

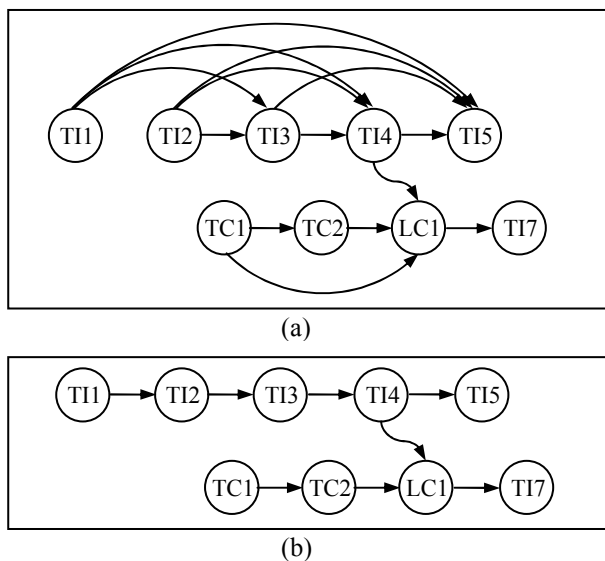


Figure 5. Digraphs considering all detected causalities (a) and after removing redundant connections (b).

Only strong connections for TC1 and LC1 were considered in an intuitive manner. The simplified digraph that omits redundant dependencies is shown in Figure 5 (b). A fault propagation path from TI1 through to TI5 can be retraced and then further on to TC1 to TI7 over TC2 and LC1. The two groups are connected only through a single arc between TI4 and LC1 which suggests that a relationship does not exist between TI5 and TC1. It is thought that the controllers damp the characteristic of the disturbance. Internal reactor characteristics coupled with temperature measurement issues may also be masking the expected relationships.

The directionality measure supports the hypothesis of an upstream disturbance rather than a problem with the level measurement. Level in the bottom tray and temperatures in the reactor are related as expected due to the nature of the reactor process. It can be concluded from the results of the directionality measure that the disturbance is not caused by the level controlled flow but by an upstream disturbance originating at a point before the reactor. The disturbance is entering at a plant boundary and is not originating within the unit. This is a significant and useful finding because it means the root cause is further upstream.

5 Conclusions

The concept of the nearest neighbor method, predictability improvement, which incorporates both time delay and attenuation, was presented here for directionality analysis. An indication can be given towards the direction of propagation and the root cause.

Guidelines derived from experimental studies are given to aid its routine implementation. In a case study of a reaction process the directionality of fault propagation was successfully investigated and gave unambiguous results. A digraph could be constructed from the directionality measure that showed the fault propagation path of the oscillatory disturbance. One of the advantages of the nearest neighbor method is the simple implementation and the generic approach. In comparison to directionality measures based on the probability density function fewer data samples are required to give consistent results. A drawback of the nearest neighbors method is that a pre-selection of variables that show similar time trends has to be undertaken to retrieve useful results. Its role in plant auditing is therefore a drill-down tool once the major disturbances have been mapped out.

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