Data-based causality analysis by exploiting process connectivity information

Rinat Landman

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Abstract

Industrial systems are often subjected to abnormal conditions due to faulty operations or external disturbances. Faults can easily propagate via the process components through material or information flows, thereby deteriorate the process performance and product quality and increase the operational costs. Therefore, it is of major importance to detect a fault, locate its root cause and reveal how it had propagated within the system.

Capturing the causality of a system has a key role in fault diagnosis due to its ability to identify the root cause of a fault and retrace its propagation path. Thus far, several data-based methods have been proposed in order to capture causality from time series corresponding to process variables. However, the majority of the data-based methods suffer from several limitations and deficiencies which compromise their ability to provide adequate results, particularly when investigating complex systems with a high level of connectivity.

This thesis proposes a hybrid causal analysis which automatically incorporates the information on the process connectivity into data-based analysis using a specialized search algorithm. The analysis aims to enhance the results accuracy, minimize the computational effort and to successfully tackle multivariate complex systems. This thesis entails four methodologies for a hybrid causal analysis based on the following causality estimators: Granger causality, transfer entropy, nearest neighbors and non-parametric multiplicative regression causality estimator. The hybrid causal analysis is successfully demonstrated on an industrial board machine using each of the causality estimators. The analysis aims to detect the propagation of an oscillatory disturbance due to valve stiction within the control loops of the drying section of the machine. Finally, the results of each causality estimator are evaluated and the methods are compared. The obtained results show that the hybrid causal analysis produced an enhanced causal model which depicts the oscillation propagation path and its root cause. Taken together, the findings of this study suggest that the connectivity information is essential for obtaining an adequate causal model when investigating complex systems. A natural progression of this work could be to implement the proposed hybrid analysis using other case studies with different types of faults.

Keywords Causality, process connectivity, fault propagation, control loops, oscillations, board machine

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Preface

The research work presented in this thesis has been carried out in the research group of Process Control and Automation, Aalto University, Department of Chemical and Metallurgical Engineering, School of Chemical Engineering, Espoo, Finland during the period 2014-2018. The research leading to these results has received funding from the School of Chemical Engineering, Aalto University and from the European Union Seventh Framework Programme (FP7/2007-2013) under grant agreement No. 257580. In addition, financial support for the research has been received from the Finnish Automation Foundation and Plantwide eMPC project of the Academy of Finland under agreement No. 13296432.

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List of Abbreviations

AAFT	Amplitude Adjusted Fourier Transform
ADF	Augmented Dicky-Fuller
AIC	Akaike Information Criterion
AR	Autoregressive
BIC	Bayesian Information Criterion
BM	Board Machine
CAD	Computer-Aided Design
CAEX	Computer Aided Engineering Exchange
CCF	Cross-Correlation Function
CFTd	Direct Causal Fourier Transform
CFTf	Full Causal Fourier Transform
CT	Condensate Tank
DCS	Distributed Control System
DFS	Depth First Search
DG	Drying Group
DTE	Direct Transfer Entropy
DTE_{diff}	Differential Direct Transfer Entropy
DTF	Directed Transfer Function
FDD	Fault Detection and Diagnosis
GC	Granger Causality
IAAFT	Iterative Amplitude Adjusted Fourier Transform
LC	Level Controller
MV	Multivariate
MVAR	Multivariate Autoregressive
NARX	Nonlinear autoregressive exogenous
NN	Nearest Neighbors
NPMR	Non-Parametric Multiplicative Regression
NDTE	Normalized Direct Transfer Entropy

$NDTE_{diff}$	Normalized Differential Direct Transfer Entropy
NTE	Normalized Transfer Entropy
NTE_{diff}	Normalized Differential Transfer Entropy
OOP	Object-Oriented Programming
OP	Control Output
PC	Pressure Controller
PDA	Plant-wide Disturbance Analysis
PDC	Partial Directed Coherence
PDF	Probability Density Function
PFD	Process Flow Diagram
PI	Pressure Indicator
P&ID	Piping and Instrumentation Diagram
PSDG	Probabilistic Signed Directed Graph
PV	Controlled Variable
QCS	Quality Control System
RMPCT	Robust Model-Predictive Control Technology
RPC	Relative Power Contribution
RSS	Residual Sum of Squares
SDG	Signed Directed Graph
SG	Steam Group
TE	Transfer Entropy
TE_{diff}	Differential Transfer Entropy
TSS	Total Sum of Squares
XML	Extensible Markup Language
WSS	Wide Sense Stationary

List of Publications

This thesis consists of a summary of the following publications which are referred to in the text by their Roman numerals.

- I Landman, R., Kortela, J., Sun, Q. and Jämsä-Jounela, S.-L. Fault propagation analysis of oscillations in control loops using data-driven causality and plant connectivity. *Computers and Chemical Engineering*, **71**, 446–456, 2014. [dx.doi.org/10.1016/j.compchemeng.2014.09.017](https://doi.org/10.1016/j.compchemeng.2014.09.017).
- II Landman, R. and Jämsä-Jounela, S.-L. Hybrid approach to causal analysis on a complex industrial system based on transfer entropy in conjunction with process connectivity information. *Control Engineering Practice*, **53**, 14–23, 2016. [dx.doi.org/10.1016/j.conengprac.2016.04.010](https://doi.org/10.1016/j.conengprac.2016.04.010).
- III Landman, R. and Jämsä-Jounela, S.-L. Fault propagation analysis by implementing nearest neighbors method using process connectivity, *IEEE Transactions on Control Systems Technology*, **PP**, 1-10, 2018. [10.1109/TCST.2018.2847651](https://doi.org/10.1109/TCST.2018.2847651).
- IV Landman, R. and Jämsä-Jounela, S.-L. Hybrid causal analysis combining a nonparametric multiplicative regression causality estimator with process connectivity information. Submitted for publication in *Control Engineering Practice* on 11.02.2019.

Author's Contribution

Publication I: The author proposed and developed the methodology of the hybrid causal analysis for combining Granger causality with the connectivity information, developed the search algorithm and the algorithms of the Granger causality and frequency domain analysis, performed all the simulations, analyzed and interpreted the results and wrote the manuscript. J. Kortela and Q. Sun extracted the process connectivity information and generated the topology-based model of the drying section of the board machine from the P&ID of the process. In addition, J. Kortela wrote on generating a topology-based model in the manuscript. Prof. Jämsä-Jounela provided guidance throughout the entire work and writing procedure.

Publication II: The author proposed and developed the hybrid causal analysis for combining the transfer entropy method with the connectivity information and designed accordingly the search algorithm. Furthermore, the author developed the transfer entropy algorithms, performed all the simulations, analyzed the results and wrote the manuscript under the supervision of Prof. Jämsä-Jounela.

Publication III: The author proposed and developed the methodology for the hybrid causal analysis combining the nearest neighbors method with the connectivity information and designed accordingly the search algorithm. Furthermore, the author implemented the nearest neighbors algorithms, proposed and developed the new directionality measure for multivariate systems, performed all the simulations, analyzed the results and wrote the manuscript under the supervision of Prof. Jämsä-Jounela.

Publication IV: The author proposed and developed the hybrid causal analysis framework based on the NPMR-based estimator and designed accordingly the search algorithm. Furthermore, the author developed and tested the algorithms

of the NPMR-based estimator, performed all the simulations, analyzed the results and wrote the manuscript under the supervision of Prof. Jämsä-Jounela.

1. Introduction

1.1 Background

Industrial systems often exhibit abnormal events such as process disturbances, faulty operations and control failures. In large-scale systems, faults can easily propagate through the process units due to material or information flows, leading to excessive energy consumption, increased operation costs, poor product quality and at times hazardous situations. Thus, it is of major concern to detect the root cause of the faulty condition and to identify the propagation of faults within the process units. Causal analysis has a key role in fault detection and diagnosis (FDD) due to its ability to capture the causal dependencies between process variables, thereby enabling the disclosure of the the root cause and propagation path of faults.

Causal analysis yields a causal model in the form a directed graph which depicts the propagation path of a fault. A directed graph is composed of nodes corresponding to process variables and arcs denoting the causal directionality (Yang et al., 2012). Causality can be captured from process knowledge and / or process data. Modeling based on process knowledge is typically based on mathematical models describing the process phenomena (e.g., differential equations) or it can be derived directly from the process flow diagram (PFD) or the piping and instrumentation diagram (P&ID) (Yang & Xiao, 2012; Yang et al., 2012). Models which are based on the process schematic are often referred to as topology-based models or process connectivity models (Di Geronimo Gil et al., 2011). Nowadays, P&IDs are readily available in a standardized electronic form (XML) using several intelligent computer-aided design (CAD) tools and the information on the plant topology can be extracted from these tools as open XML text describing the process connectivity. Although CAD tools offer a practical method for automated causal analysis, the connectivity information is merely a

qualitative representation of the process schematic which does not include any information on the process itself (Yim et al., 2006).

On the other hand, data-based methods for capturing causality utilize historical process data in the form of time-series in order to measure to what extent the time series corresponding to the process variables influence each other. As such, they provide a practical tool for obtaining useful insights into the process dynamics with minimal effort, particularly when process knowledge is limited or unavailable. Data-based methods exploit features such as time-delays, oscillations, conditional probabilities and information transfer in order to provide a quantitative measure of causality between two variables (Yang & Xiao, 2012). Data-based methods for capturing causality can be roughly classified into two categories: linear and non-linear. Common linear methods include cross-correlation analysis (Bauer & Thornhill, 2008), Granger causality (Bressler & Seth, 2011; Granger, 1969) and frequency domain measures such as directed transfer function (DTF) (Kaminski & Blinowska, 1991) and partial directed coherence (PDC) (Baccala & Sameshima, 2001). The DTF and PDC are the normalized measures of the total and direct energy transfer, respectively, between two variables in a multivariate process (Yang & Xiao, 2012). Non-linear methods include transfer entropy (Bauer et al., 2007a; Schreiber, 2000), nearest neighbors (Bauer et al., 2005a, 2007b) and Bayesian networks (Yang & Xiao, 2006). Typically, data-based analysis yields quantitative directionality measures which are stored in a causality matrix, ultimately containing the structural information of the causal model.

Each of the data-based methods for capturing causality has its own limitations which should be considered based on the investigated system and fault type. Most of the linear methods are parametric, rely on model fitting and are restricted to linear causality which is rarely present in complex industrial systems (Yang & Xiao, 2012). On the other hand, non-linear methods such as transfer entropy require more computational effort than the linear methods (Duan et al., 2013). Furthermore, the majority of the data-based methods are based on pairwise analysis, thus, they are not able to distinguish between direct and indirect causality. Consequently, several extensions to the data-based methods have been proposed in order to handle non-linearity or / and multivariate systems. For example, Chen et al. (2004) proposed the conditional extended Granger causality and Duan et al. (2013) introduced the direct transfer entropy (DTE) in order to distinguish between direct and indirect causal relations in a multivariate nonlinear system. However, these approaches require a large amount of data in order to provide reliable results and their computational complexity is high.

Faes et al. (2008a) proposed a new approach to assess Granger causality in short bivariate series by using a nonlinear autoregressive exogenous (NARX) model. However, this approach is limited to bivariate analysis and up to a 3rd order nonlinearity. Therefore, it seems that in order to tackle large-scale complex systems while retaining a reasonable computational effort, the results should be validated by another method or by process knowledge.

Consequently, several attempts have been made to combine data-based causal analysis with plant-topology models. For instance, Yang et al. (2010b, 2012) applied TE and cross-correlation analysis in order to validate a causal model based on process knowledge and vice versa. Furthermore, Thambirajah et al. (2007, 2009) introduced a cause-and-effect analyzer combining the connectivity information of a process with the results obtained from data-based causality analysis. The fundamental idea behind the analyzer is to reduce the number of spurious results by searching for feasible propagation paths from the suspected root causes of the disturbance to all the other measurement points affected by the root cause. The possibility to automatically capture the plant topology as Computer Aided Engineering Exchange (CAEX) schema and link it with a data-driven causal analysis using a search algorithm provides a vital tool for root cause diagnosis and process insights for industrial applications (Thambirajah et al., 2007, 2009; Yang et al., 2014; Yim et al., 2006). However, finding feasible propagation paths among process components might not be sufficient in order to capture the causality of complex systems. Therefore, it remains a challenge to develop an efficient diagnostic tool which is able to tackle a highly inter-connected system with a reasonable level of veracity.

1.2 Research problem and asserted hypothesis

The majority of the data-based methods are restricted to bivariate analysis, per se, they cannot capture the true causality of a process. Thus, often it is impossible to distinguish between direct and indirect interactions without additional information (Yang & Xiao, 2012). Moreover, the ability to discriminate between direct and indirect connectivity is essential when analyzing industrial systems which are deeply inter-connected.

In recent years, several extensions have been proposed to Granger causality (GC) such as the extended GC (Chen et al., 2004) and partial GC (Guo et al., 2008). However, the GC and its extensions rely on autoregressive modelling, therefore they might not be applicable to highly non-linear processes. In addition, a number of studies have proposed modifications and extensions to TE. For instance, Shu

& Zhao (2013) introduced a modification to TE by improving the estimation of the time delay based on the prediction horizon. Vakorin et al. (2009) proposed the partial TE which considers the effect of indirect causality in a multivariate environment. However, the partial TE considers all the environmental variables to be intermediate which is not necessarily true in chemical processes. Duan et al. (2014b) proposed the transfer 0-entropy on the basis of the definitions of 0-entropy and 0-information as a new measure for causality while Duan et al. (2013) suggested the DTE which discriminates between direct and indirect causality in a multivariate system. Although TE and its extensions are nonlinear, their implementation requires a considerably high computational effort for estimating the probability density functions (PDF). Thus, there is a tradeoff between the accuracy of the results and the computational burden which should be taken into account when selecting the parameters for the TE estimation (Duan et al., 2013).

Consequently, there is a growing need for developing a causal analysis which is able to tackle complex systems while offering an efficient and practical tool for identifying the propagation path and root cause of faults. This thesis addresses that need by developing a hybrid causal analysis which combines data-based methods with information on the process connectivity in order to retrace the propagation path of a disturbance within control loops. The process connectivity information is automatically incorporated into the causal analysis using a specialized search algorithm which enables the determination of the type of connectivity between each pair of controllers in a system. Thereby, this type of hybrid causal analysis provides an enhanced and powerful diagnostic tool which is suitable for industrial applications. The work focuses on an industrial board making process, in particular, its drying section which exemplifies a highly inter-connected system.

The hypothesis asserted in this thesis is :

A hybrid causal analysis which automatically integrates information on the process connectivity with data-based methods provides an enhanced causal model which can serve as a basis for the development of a powerful FDD system.

To prove the claims of the hypothesis presented above, the following tasks were carried out throughout the research:

Task 1.

Four hybrid causal analysis methodologies were developed that combine a

topology-based model with various data-based causality estimators using a specialized search algorithm. The integration of the connectivity information with the causality estimators is carried out by taking into account the intrinsic features of each estimator. The developed causal analysis methods aim to discriminate between direct and indirect causality, hence, producing efficient and practical tools for fault propagation and root cause analysis in systems with a high level of connectivity.

Task 2. A unique search algorithm based on a depth-first search (DFS) was developed in order to combine a topology-based model with data-based causal analysis for identifying the propagation path of a disturbance through control loops. The algorithm was primarily designed to execute the following consecutive tasks: first, it determines whether feasible propagation paths between each pair of controllers exist. Then, if such paths exist, the algorithm checks whether each path is direct or indirect based on the process topology using the connectivity matrix.

Task 3.

A new multivariate extension to the nearest neighbors method was proposed in order to distinguish between direct and indirect causality in a nonlinear multivariate system.

Task 4.

The proposed methodologies for hybrid causal analysis were implemented on an industrial board machine aiming to identify the propagation of an oscillatory disturbance through the control loops of the drying section of the machine. The performance of each causality estimator was evaluated and the estimators were compared. In addition, guidelines for selecting the most appropriate estimator based on the investigated system and fault were provided.

1.3 Scope and significance of the thesis work

This thesis is focused on developing a hybrid causal analysis that can retrace the propagation path and root cause of faults by exploiting both process data and connectivity information. CAD tools that can easily capture the connectivity information from process schematics offer a practical and efficient way to perform automated causal analysis. Furthermore, typically process data is readily available in modern industrial systems and is a valuable source for modeling and analysis. The utilization of a search algorithm to automatically incorporate

the connectivity information with data-based causal analysis is an important step in the implementation of FDD methods for industrial systems in the future.

The main contribution of this thesis is the development of a hybrid causal analysis for retracing the propagation path of faults within control loops by utilizing a unique DFS algorithm. The search algorithm is the keystone of the analysis due to its ability to discriminate between direct and indirect physical connectivity based on the process topology. Ergo, the causality is estimated based on the type of physical directionality. Consequently, the hybrid causal analysis can efficiently deal with multivariate industrial systems and simultaneously reduce the computational burden. Four methodologies for causal analysis using several linear and non-linear causality estimators have been developed by taking into account the inherent characteristics of each estimator. Thereby, the proposed hybrid approach for causal analysis can serve as a basis for the future development of a powerful diagnostic tool for industrial applications. Each causal methodology is demonstrated on a drying section of an industrial board machine with multiple oscillating control loops due to valve stiction.

The novelty of the thesis is demonstrated in the four publications presented and demonstrate the hybrid causal analysis using various causality estimators. Publication I presents a hybrid causal analysis which utilizes the information on the process connectivity in order to validate the results of the GC method. In addition, it illustrates how the frequency domain methods can be used to verify the results of a causal analysis and to identify the root cause of a fault. Publication II presents a hybrid causal analysis by combining the TE method with process connectivity information. The analysis entails both bivariate and multivariate directionality measures which are implemented in two phases. The search algorithm is utilized in both phases in order to incorporate the connectivity information. Publication III proposes a two-phase methodology for hybrid causal analysis using the nearest neighbors method in conjunction with the process connectivity information. In phase I, the bivariate directionality measure is calculated only for the paths which are considered as direct based on the process topology. In phase II, a new multivariate directionality measure is introduced in order to exclude indirect pathways from the causal model. Publication IV proposes a hybrid methodology for non-linear causal analysis based on non-parametric multiplicative regression (NPMR) for detecting the propagation path of disturbances in control loops. The estimator is applied to both pairwise and multivariate estimations while the connectivity information is automatically integrated into the analysis by utilizing the search algorithm.

Outside of the thesis scope are fault detection analysis, corrective actions such as

fault accommodation using fault tolerant control as well as software engineering aspects of the implementation of the developed methodology in industrial systems.

1.4 Outline of the thesis

This thesis is organized as follows. Chapter 2 presents the state-of-the-art of capturing causality in industrial systems. First, the concepts of connectivity and causality are discussed. Next, data-based methods for capturing causality are described and the procedure for extracting plant connectivity from process schematic is explained in detail. In addition, techniques for combining data-based and topology-based models are discussed. The developed hybrid causal analysis for each causality estimator is described and illustrated in Chapter 3. The drying section of the paperboard machine and the case study are described in Chapter 4. Chapter 5 presents the results of the hybrid causal analysis using each of the causality estimators. Then, the estimators are compared and evaluated based on the characteristics and outcome of each method. The thesis ends with summary and conclusions in Chapter 6.

2. Capturing process causality in industrial systems; State-of-the-art

This chapter presents the state-of-the-art of capturing causality in industrial systems. First, the concepts of connectivity and causality are introduced. Next, capturing causality from process knowledge is briefly described. In particular, the procedure for extracting the plant topology from P&ID is discussed. Then, a survey of the relevant literature on the data-based methods for capturing causality is presented. Lastly, several techniques for combining data-based and topology-based models for mutual validation of causal analysis are discussed.

2.1 Introduction to the concept of causality

Large-scale systems are characterized by causality which is a physical phenomena based on a cause-effect relationship between different variables (Pearl, 2009). Typically, when a fault occurs in industrial system it can easily propagate through the process components due to material or information flows, causing the process to deviate from its desired operating conditions (Yang & Xiao, 2012). Detection of the root cause of a fault by human labor is usually time consuming, difficult and expensive. Those considerations motivate the study of causal relationships between process variables which will enable the identification of propagation paths of faults and hereby detect their root cause.

Causality is based upon two other conditions: connectivity and correlation. However, correlation and connectivity do not necessarily imply causality. For instance, two vessels can be connected via a pipe with a closed valve, thus, there is no material flow between the vessels and therefore no causal dependency. Another case is when two variables are correlated since they are driven by a third variable, however, there is no causality between the two variables since they do not influence each other. Similarly, if two variables are interacting via an intermediate variable, they might be correlated but the causality between them is indirect. Hence, there is a major difference between direct and indirect

causality. When trying to reveal the propagation path of a fault, one must capture accurately the process topology by identifying the direct causality between the process variables. Therefore, identification of direct causality in a multivariate environment with a large number of variables is a well-known problem in causality analysis (Yang & Xiao, 2012; Yang et al., 2014).

Another important difference between causality and correlation is directionality. Correlation does not have directionality while causality does. Connectivity on the other hand, can be directed or undirected, depending on the connected path. (Yang & Xiao, 2012). Establishing connectivity and causality of industrial processes enables the capturing of the process topology which, in turn, can assist in various diagnostic applications.

2.2 Capturing topology from process knowledge

Process knowledge is considered as the most reliable resource for capturing the topology of a complex process and it includes process schematics and expert knowledge stored in human brains (Yang et al., 2014). Models based on process knowledge can be based on first principles mathematical equations (e.g., differential equations, algebraic equations) describing the process phenomena (Yang & Xiao, 2012; Yang et al., 2014). This type of model is usually represented as a digraph or a signed digraph (SDG) illustrating the positive or negative influences between the variables (Di Geronimo Gil et al., 2011). Several methods have been developed for generating SDGs from various mathematical models and for SDG analysis predicting the initial or steady state response of a system to external disturbances (Maurya et al., 2003, 2004). Alternatively, a qualitative model can be established directly from process schematics. These models are typically referred to as topology-based models or process connectivity models (Di Geronimo Gil et al., 2011).

Connectivity describes a physical linkage between process units and the main resources for establishing connectivity are PFDs and P&IDs (Yang & Xiao, 2012). The extracted connectivity information is converted into a causal digraph or a connectivity matrix which are graphical and numerical representations of the process topology, respectively (Sun, 2013). The connectivity matrix (also referred to as an adjacency matrix (Jiang et al., 2008; Yang & Xiao, 2012)) is a binary matrix whose entries are set to '1' in case of a direct connectivity from the row element to the column element and otherwise '0' (Sun, 2013; Thambirajah et al., 2009). As an alternative to the connectivity matrix, the variables in the causal digraph are expressed as nodes and each '1' entry in the connectivity matrix is

expressed as an arc linking the nodes corresponding to the two indices in the connectivity matrix (Yang & Xiao, 2012).

2.2.1 Extracting connectivity information from a process schematic

Connectivity information can be easily exported from a process schematic using computer aided engineering tools such as AutoCAD P&ID, SmartPlant P&ID and ComosPT in the form of Extensible Markup Language (XML) or XLS/XLSX (Microsoft Excel file format) (Sun, 2013). XML is a scripting language that describes the equipment, their properties and the connections among them while ensuring it can be interpreted by humans and computers (Yim et al., 2006; Thambirajah et al., 2009).

In this study, the connectivity information was exported using the AutoCAD P&ID drafting application which has been developed based on Autodesk AutoCAD (publication I). The AutoCAD P&ID consists of comprehensive P&ID symbol libraries which cover a wide range of standards such as PIP, ISA, ISO and DIN. Two accepted schemes, Computer Aided Engineering Exchange (CAEX) and XMpLant define XML syntax when using XML files to represent plant topology (Thambirajah et al., 2009). In the developed application, the topology data was exported in the format of ISO 15926-compliant XML scheme XMpLant (Laud, 2010; Sun, 2013). XMpLant is an XML standard which can be used to map data in a specific proprietary software to a format of ISO 15926 and then transfer it to any other desirable proprietary system (Laud, 2010). The XMpLant schema defines a specific XML structure which supports all required process engineering information, including process objects, topology and geometry. (Sun, 2013; Laud, 2010).

The automated generation of the connectivity information is performed in three steps as indicated in Figure 2.1. The first step is carried out by the P&ID software while the causal models are generated using Object-Oriented Programming (OOP) in the second and third step (Sun, 2013).

First, all the information on the line segments and their initial and terminal components (e.g., tanks, valves, instruments) is drawn in a new drawing using the Project Setup Wizard. Each component is given a specific tag name based on its type in order to distinguish the components from each other. The new drawing is built based on the original AutoCAD drawing which is used as a reference. Once the drawing is finished, all the topology information can be extracted through the database object of the drawing. Namely, all the names of the process components, their coordinates and the connections among them can be exported as an XML report. (Sun, 2013)

Figure 2.1. The procedure of generating topology-based model (Sun, 2013)

Finally, this information is further processed using MATLAB and converted into a topology-based model. The generation of the model is performed by MATLAB OOP which considers the task as a class and defines the topology-data as static characteristics (called Properties) and the steps for developing the model as dynamic characteristics (called Methods). The OOP consists of three steps: classification of the problem, definition of the class and instantiation of the class. Since both causal models (the digraph and the connectivity matrix) can be obtained from the same topology information, the generation of both models is classified as one group. In the second step, static and dynamic characteristics of the object are explored and generalized to a class. The static characteristics include the names of the components, their coordinates and directionality. The dynamic characteristics define the function to develop the causal model. For instance, the functions 'getMatrix' and 'digraph' are used to generate the connectivity matrix and the causal digraph, respectively. Finally, in step 3 the topology information is imported into a defined class which is instantiated to a specific object by assigning values to its properties (Sun, 2013).

2.3 Capturing causality from process data

Process data in the form of time series is a valuable resource for fault detection and diagnosis applications. When a fault propagates through a system, it changes the dynamics of the process, and thus, specific features such as time delay, oscillations, conditional probabilities and signal attenuation can be used to retrace

Figure 2.2. Data-based methods for capturing causality and their classification

the propagation path. Data-based methods exploit those features in order to provide a quantitative measure of causality between time series (Yang & Xiao, 2012). Several classifications have been proposed for data-based methods (Yang & Xiao, 2012; Yang et al., 2014), however, for simplicity, in this thesis the methods are classified into two categories: linear and non-linear. Figure 2.2 presents the data-based methods which are reviewed in this thesis and their classification.

For each method, a short description is given including a mathematical formulation. In addition, the parameters settings and evaluation of the statistical significance of the results are discussed.

2.3.1 Linear methods

Cross-correlation analysis

The cross-correlation method exploits the time delays between measurements and offers a model-free causal analysis. As aforesaid, correlation does not necessarily imply causality, however, time-delayed correlation can be taken as evidence for causality since time delays are due to physical causation (Bauer & Thornhill, 2008). The cross-correlation function (CCF) between two time series with N observations and a lag k is :

$$\phi_{xy}[k] = \begin{cases} \frac{1}{N-k} \sum_{i=1}^{N-k} \hat{x}_i \hat{y}_{i+k}, & k \geq 0 \\ \frac{1}{N+k} \sum_{i=1-k}^N \hat{x}_i \hat{y}_{i+k}, & k \leq 0 \end{cases} \quad (2.1)$$

where $\hat{x}_i$ and $\hat{y}_i$ are scaled by removing the mean and scaling to a unit standard deviation. The time delay, λ , is equal to k at which the CCF gets its maximum absolute value. The estimation of λ is derived by calculating both the minimum and maximum of the CCF as follows:

$$\phi^{max} = \max\{\phi_{xy}(k^{max})\}, \quad \phi^{min} = \min\{\phi_{xy}(k^{min})\} \quad (2.2)$$

The time delay is defined as:

$$\lambda = \begin{cases} k^{max}, & \phi^{max} \geq -\phi^{min} \\ k^{min}, & \phi^{max} \leq -\phi^{min} \end{cases} \quad (2.3)$$

If $\lambda > 0$ it means that y is delayed by k^{max} and if $\lambda < 0$, the delay is from y to x . The maximum time delayed correlation between two series is defined as (Bauer & Thornhill, 2008):

$$\rho = \max\{\phi^{max}, |\phi^{min}|\} \quad (2.4)$$

The sign of ρ corresponds to the sign of the arc in the SDG.

The *directionality index* (Bauer & Thornhill, 2008) which measures the difference between the minimum and maximum of $\phi_{xy}[k]$ is defined as

$$\psi = 2 \frac{|\phi^{max} + \phi^{min}|}{\phi^{max} + |\phi^{min}|} \quad (2.5)$$

Bauer & Thornhill (2008) proposed a method for selecting the threshold for the significance testing of the correlation coefficient and the directionality index. The selection is based upon determining the empirical distribution of ρ and ψ for varying number of samples, N , under the null hypothesis of no causal relationship between x and y .

In addition, Bauer & Thornhill (2008) proposed a procedure for capturing the process topology based on the time-delay estimation. Initially, a causality matrix is obtained based on the estimated time-delay. Then, each entry in the causality matrix undergoes a consistency check in order to verify the results. Finally, the causal model is derived from the verified causality matrix by considering two alternative topologies.

Tangirala et al. (2005) introduced the power spectral correlation map for clustering variables with similar spectral features. This provides a useful tool of visualizing correlation, especially for the identification of small groups of variables (Yang et al., 2014).

The cross-correlation method offers a practical and a straightforward approach for identifying causality, however, it suffers from several limitations when considering

industrial applications:

- Non-linear causal relationships do not necessarily appear in the correlation analysis (Yang et al., 2012).
- Some physical properties like temperature and composition travel with a significant delay while others like variations in pressure or flow of incompressible fluids are almost instantaneous. The latter can be problematic if the delay is negligible compared with the sampling time. (Bauer & Thornhill, 2008)
- When time series exhibit harmonic oscillations, the resulting CCF is periodic with the same frequency as the oscillations. Thus, it is not possible to determine whether the delay is from x to y or vice versa (Bauer & Thornhill, 2008).
- Correlation analysis simply provides an estimate of the time delay while the sign of the delay is an estimate of the directionality of the flow. In addition, variations in time series are ignored and values at different time instances are regarded as samples of the same event (Yang et al., 2014).
- The method is implemented as a pairwise analysis. Thus, it might not be applicable to highly inter-connected systems with many variables. Furthermore, any other related variables can affect the correlation between two given variables, thus, process knowledge should be taken into account to identify the topology of a correlated group of variables (Yang et al., 2014).

Granger causality method

Granger causality has received much attention in many areas such as neuroscience, biology and economics due to its straightforward approach and efficiency when investigating causal dependencies (Bressler & Seth, 2011; Seth, 2005; Yuan & Qin, 2013). The notion for GC was first introduced by Wiener (Wiener, 1956) and was later formulated by Granger (Granger, 1969). The basic notion of GC is that if one series affects another series, then the past information of the former series should help to predict the future of the latter one (Granger, 1969). This idea can be expressed via a linear regression model. Namely, if the incorporation of the past measurements from one series reduces the variance of the prediction error of a second series, then one can conclude that the first series has a causal effect on the second one. Consider two series $X_1(t)$ and $X_2(t)$ and

their corresponding autoregressive (AR) model:

$$\begin{aligned} X_1(t) &= \sum_{j=1}^p A_{1,j} X_1(t-j) + \epsilon'_1(t) \\ X_2(t) &= \sum_{j=1}^p A_{2,j} X_2(t-j) + \epsilon'_2(t) \end{aligned} \quad (2.6)$$

Jointly, they can be represented as:

$$\begin{aligned} X_1(t) &= \sum_{j=1}^p A_{11,j} X_1(t-j) + \sum_{j=1}^p A_{12,j} X_2(t-j) + \epsilon_1(t) \\ X_2(t) &= \sum_{j=1}^p A_{21,j} X_1(t-j) + \sum_{j=1}^p A_{22,j} X_2(t-j) + \epsilon_2(t) \end{aligned} \quad (2.7)$$

where p is the model order and $\epsilon'_1(t), \epsilon'_2(t), \epsilon_1(t), \epsilon_2(t)$ are the residuals. Eq. 2.6 is typically referred to as the *restricted model* and Eq. 2.7 is referred to as the *unrestricted model* (Bressler & Seth, 2011). The GC from $X_2(t)$ to $X_1(t)$ is defined as (Seth, 2010):

$$F_{x_2 \rightarrow x_1} = \ln \left[\frac{\text{var}(\epsilon'_1)}{\text{var}(\epsilon_1)} \right] \quad (2.8)$$

The statistical significance can be determined via the F -statistic test (Greene, 2002)

$$F = \frac{RSS_r - RSS_{ur}}{RSS_{ur}} \times \frac{T - 2p - 1}{p} \quad (2.9)$$

where RSS_r and RSS_{ur} are the residual sum of squares of the *restricted* and *unrestricted* models respectively and T is the total number of observations. A significant F -statistic can be interpreted as evidence that the *unrestricted* model provides a better prediction than the *restricted* model, thus, $X_2(t)$ *G-causes* $X_1(t)$ (Bressler & Seth, 2011).

GC can be generalized for multivariate (MV) (conditional) systems by including in the AR model multiple additional variables (Geweke, 1982). In this case, $X_2(t)$ *G-causes* $X_1(t)$ if $X_2(t)$ reduces the variance of the prediction error of $X_1(t)$ when all the other variables are included in the AR model (Seth, 2010). For example, consider a system of three variables: $X_1(t), X_2(t), X_3(t)$. The conditional GC from $X_2(t)$ to $X_1(t)$ can be obtained from the following *restricted* and *unrestricted*

models by including $X_3(t)$ in Eqs. 2.6-2.7, respectively:

$$\begin{aligned} X_1(t) &= \sum_{j=1}^p B_{1,j} X_1(t-j) + \sum_{j=1}^p B_{3,j} X_3(t-j) + \epsilon'_3(t) \\ X_1(t) &= \sum_{j=1}^p B_{11,j} X_1(t-j) + \sum_{j=1}^p B_{12,j} X_2(t-j) + \sum_{j=1}^p B_{13,j} X_3(t-j) + \epsilon_3(t) \end{aligned} \quad (2.10)$$

Then, the GC from $X_2(t)$ to $X_1(t)$ conditional on $X_3(t)$ can be calculated as follows:

$$F_{x_2 \rightarrow x_1 | x_3} = \ln \left[\frac{\text{var}(\epsilon'_3)}{\text{var}(\epsilon_3)} \right] \quad (2.11)$$

Geweke (1982, 1984) made an important contribution to the area by developing a spectral decomposition of the GC by examining the Fourier components of a multivariate autoregressive (MVAR) model in the time domain.

The GC method requires the series to be stochastic and wide sense stationary (WSS) in order to produce adequate results (Granger & Newbold, 1974). Non-stationary data might indicate that the relations vary with time. In this case, one could use recursive least squares modeling. The estimation of AR models requires an estimate of the model order (p). A very low order can lead to poor estimation while a very high order can lead to overfitting. An acceptable model order should produce residuals which are close enough to white noise (Bressler & Seth, 2011). Two criteria are suitable when selecting the model order: The Akaike information criterion (AIC) (Akaike, 1974) and the Bayesian information criterion (BIC) (Schwartz, 1978).

In summary, the GC is a practical method with an acceptable computational burden which has been widely used in many applications (Yuan & Qin, 2013). However, both GC and its extensions are based on AR models, thus, its application to nonlinear systems may be inappropriate (Bressler & Seth, 2011). Moreover, the model accuracy directly affects the reliability of the results. Thus, the model order and the number of observations should be carefully considered.

In some cases, especially those dealing with large-scale systems, linear approximations were found to work very well (McIntosh & Gonzalez-Lima, 1994). Specific implementations of the non-linear GC include a kernel based method (Ancona et al., 2004; Chen et al., 2017; Marinazzo et al., 2008). However, multivariate cases are not discussed in those studies.

Frequency domain methods

Frequency domain methods can be seen as a decomposition of the energy transfer between time series at each frequency. Frequency domain analysis can reveal the direction of energy transfer, quantify it and distinguish between direct and indirect interactions. The evaluation of causal relations in the frequency domain is especially useful for a process with oscillatory behavior (Faes et al., 2010). All the methods are based on AR models converted via Fourier transform into frequency domain. An MVAR model is defined as :

$$\begin{bmatrix} x_1(t) \\ \vdots \\ x_N(t) \end{bmatrix} = \sum_{r=1}^p A_r \begin{bmatrix} x_1(t-r) \\ \vdots \\ x_N(t-r) \end{bmatrix} + \begin{bmatrix} e_1(t) \\ \vdots \\ e_N(t) \end{bmatrix} \quad (2.12)$$

where $X_t = [x_1(t), x_2(t), \dots, x_N(t)]$ is the vector of N process variables, $E_t = [e_1(t), e_2(t), \dots, e_N(t)]$ is N dimensional vector of the MV zero mean uncorrelated white noise, $A_1, A_2, \dots, A_p$ are $N \times N$ matrices of the model coefficients and p is the model order. The Z transform operator is defined as :

$$Z^{-i} = e^{-i2\pi f j} \quad (2.13)$$

By applying the Z transform operation to Eq. 2.12, it is transformed into frequency domain:

$$X(f) = H(f)E(f) \quad (2.14)$$

where $H(f)$ is the transfer function of the MVAR model with the following relation to the model coefficients:

$$H(f) = (I - A(f))^{-1} = \bar{A}(f)^{-1} = (I - \sum_{r=1}^p A_r Z^{-r})^{-1} \quad (2.15)$$

Σ is the noise covariance matrix of the model and is defined as:

$$\Sigma = \begin{bmatrix} \sigma_{11}^2 & \cdots & \sigma_{1N} \\ \vdots & \ddots & \vdots \\ \sigma_{N1} & \cdots & \sigma_{NN}^2 \end{bmatrix} \quad (2.16)$$

where σ refers to covariance and σ^2 to the variance of the noise terms. Since it is assumed that the noise terms are uncorrelated, σ is a constant diagonal matrix and not frequency dependent. Several methods have been developed based on the

transformation of MVAR models to the frequency domain. Kaminski & Blinowska (1991) introduced the directed transfer function (DTF) which is defined as :

$$\gamma_{ij}(f) = \frac{H_{ij}(f)}{\sqrt{\sum_{j=1}^N |H_{ij}(f)|^2}} \quad (2.17)$$

The DTF represents the normalized measure of the power contribution from x_j to x_i through both direct and indirect pathways. The DTF has the following properties: $0 \leq |\gamma_{ij}(f)|^2 \leq 1$ and $\sum_{j=1}^N |\gamma_{ij}(f)|^2 = 1$. Seeing that the DTF disregards the noise terms, the estimator is not influenced if the noise terms are correlated. Furthermore, since it is assumed that the noise is uncorrelated with the signals, the transfer function is also independent of the noise. Kaminski & Blinowska (1991) have shown that the DTF is able to detect directionality between time series even if the amplitude of the noise is several times bigger than the signal itself. On the other hand, the partial directed coherence (PDC) (Baccala & Sameshima, 2001) measures only the direct causal contribution from x_j to x_i and it is defined solely from $\bar{A}_{ij}(f)$:

$$\pi_{ij}(f) = \frac{\bar{A}_{ij}(f)}{\sqrt{\sum_{i=1}^N |\bar{A}_{ij}(f)|^2}} \quad (2.18)$$

Similarly to the DTF, the normalization of the PDC yields the properties :

$0 \leq |\pi_{ij}(f)|^2 \leq 1$ and $\sum_{i=1}^N |\pi_{ij}(f)|^2 = 1$. The PDC depends on the $\bar{A}_{ij}$ coefficients which describe relationships between the present time series x_i and the past of x_j . Per se, by forsaking the Σ term from the PDC, it can be seen as the frequency domain representation of the GC (Baccala & Sameshima, 2001). Thus, it can efficiently complement time domain GC.

Winterhalder et al. (2005) have shown that if the diagonal terms of the noise covariance matrix differ by orders of magnitude, false detection of influence from a low variance variable to a high variance variable is caused. Consequently, Baccala et al. (2007) proposed a modified definition for the PDC where the model coefficients are scaled using the diagonal terms of Σ :

$$\pi_{ij}(f) = \frac{\frac{1}{\sigma_{ii}} \bar{A}_{ij}(f)}{\sqrt{\sum_{i=1}^N \frac{1}{\sigma_{ii}^2} |\bar{A}_{ij}(f)|^2}} \quad (2.19)$$

Analogously, by accounting for the noise variances, the relative power contribution (RPC) (Akaike, 1968; Yameshita et al., 2005) represents the DTF in a scaled domain:

$$r_{ij}(f) = \frac{\sigma_{jj} H_{ij}(f)}{\sqrt{\sum_{j=1}^N \sigma_{jj}^2 |H_{ij}(f)|^2}} \quad (2.20)$$

In summary, both the PDC and the DTF describe the signal power that spreads from one variable to another, however, the DTF measures the total effect of one variable on the other while the PDC measures direct effects, therefore it is more suitable for capturing the process topology. Moreover, the DTF and GC are different descriptions of relationships while the PDC coincides with the concept of GC. Gigi & Tangirala (2010) have shown that the total energy transfer between variables does not only involve direct and indirect interactions but also an interference effect due to a phase difference between the direct and indirect pathways. The total energy transfer can be represented by the DTF, however, the PDC contains the structural information of the direct influences but not the direct energy transfer itself (Gigi & Tangirala, 2010).

Typically, for visualization purposes the PDC/DTF are plotted in a matrix layout along with their threshold value at each frequency. Several techniques have been proposed for determining the statistical significance of the PDC and the DTF (Schelter et al., 2005; Takahashi et al., 2007). In this work, the statistical significance of the PDC and the DTF was determined based on the direct causal Fourier transform (CFTd) and the full causal Fourier transform (CFTf) surrogates, respectively (Faes et al., 2010). The frequency domain methods have similar advantages and limitations as GC, however, they provide better insight for the energy transfer at different frequencies (Yang & Xiao, 2012).

2.3.2 Non-linear methods

Transfer entropy

Transfer entropy (TE) is an information theoretic method proposed by Schreiber (2000) that quantifies statistical coherence between systems involved in time by measuring reduction of uncertainty. Namely, the TE measures the improvement in the prediction of y using the past values of x and y compared with past values of y alone. Consequently, it enables the identification of the direction of fault propagation and its root cause without having to require the time delay.

The TE from a stationary series x to y is defined as (Yang et al., 2012) :

$$t(x|y) = \sum_{y_{i+h}, y_i, x_i} p(y_{i+h}, y_i, x_i) \log \frac{p(y_{i+h}|y_i^k, x_i^l)}{p(y_{i+h}|y_i^k)} \quad (2.21)$$

where p is the complete or conditional PDF,

$y_i^k = [y_i, y_{i-\tau}, \dots, y_{i-(k-1)\tau}]$ and $x_i^l = [x_i, x_{i-\tau}, \dots, x_{i-(l-1)\tau}]$ denote an embedding vectors with elements from the past values of y and x , respectively (k and l are the embedding dimensions of y and x , respectively). τ is the sampling period and h is the prediction horizon.

The embedding dimensions k and l should be chosen carefully: the computational effort increases with the power of k and l as well as the number of samples required to estimate the joint PDFs. Past experience suggests that $h = \tau \leq 4$ can be used for an initial trial (Bauer et al., 2007a; Yang et al., 2012) and then the results are tested for different values of k and l (Duan et al., 2013). The selected embedding dimensions are the minimum values above which the change rate of the TE does not vary significantly. If the dead time between measurements is known, the optimum of both τ and h are equal to the dead time.

If two directions are considered, then

$$t_{x \rightarrow y} = t(y|x) - t(x|y) \quad (2.22)$$

can be used as a causality measure. Positive values of $t_{x \rightarrow y}$ indicate that x causes y while negative values indicate the opposite case. The traditional TE method is only suitable for bivariate analysis. When investigating complex systems with a large number of variables, it is essential to distinguish between direct and indirect pathways in order to capture the process topology. Duan et al. (2013) introduced the direct transfer entropy (DTE) in order to distinguish between direct and indirect pathways of information. Since we consider continuous processes, this study focuses on the differential TE (TE_{diff}) and DTE (DTE_{diff}). The TE_{diff} is defined as follows:

$$T_{x \rightarrow y} = \int f(y_{i+h1}, y_i^{k1}, x_i^{l1}) \cdot \log \frac{f(y_{i+h1}|y_i^{k1}, x_i^{l1})}{f(y_{i+h1}|y_i^{k1})} dw \quad (2.23)$$

where $f(y_{i+h1}, y_i^{k1}, x_i^{l1})$ is the joint PDF, and $f(\cdot|\cdot)$ denotes the conditional PDF. The base of the logarithm is 2 and w denotes the random vector $[y_{i+h1}, y_i^{k1}, x_i^{l1}]$ (Duan et al., 2013).

Similarly, the TE_{diff} from z to y is defined as :

$$T_{z \rightarrow y} = \int f(y_{i+h3}, y_i^{k2}, z_i^{m2}) \cdot \log \frac{f(y_{i+h3}|y_i^{k2}, z_i^{m2})}{f(y_{i+h3}|y_i^{k2})} d\zeta \quad (2.24)$$

The differential DTE (DTE_{diff}) from x to y via the intermediate variable z is

defined as :

$$D_{x \rightarrow y} = \int f(y_{i+h}, y_i^k, z_{i+h-h_3}^{m_2}, x_{i+h-h_1}^{l_1}) \cdot \log \frac{f(y_{i+h}|y_i^k, z_{i+h-h_3}^{m_2}, x_{i+h-h_1}^{l_1})}{f(y_{i+h}|y_i^k, z_{i+h-h_1}^{m_2})} dv \quad (2.25)$$

where v denotes the random vector $[y_{i+h}, y_i^k, z_{i+h-h_3}^{m_2}, x_{i+h-h_1}^{l_1}]$. The prediction horizon is set to be $h = \max(h_1, h_3)$. If $h = h_1$ then $y_i^k = y_i^{k_1}$ and if $h = h_3$, then $y_i^k = y_i^{k_2}$ (Duan et al., 2013).

The DTE_{diff} represents the future information about y obtained from past values of both x and z , after eliminating the information about the future of y from the past values of z alone (Duan et al., 2013). If this measure is greater than zero, it can be concluded that there is a direct causality from x to y . The DTE can be extended to multiple intermediate variables : $z_1, z_2, z_3, \dots, z_q$. The calculation is done according to Eq. 2.25 by considering the q -dimensional vector $[z_{1,i_1}^{s_1}, z_{2,i_2}^{s_2}, \dots, z_{q,i_q}^{s_q}]$ as the intermediate variable. The embedding dimensions $s_1, s_2, \dots, s_q$ and the time intervals $i_1, i_2, \dots, i_q$ are determined by calculating the TE from $z_1, z_2, \dots, z_q$ to y . Hence, the inclusion of intermediate variables in the DTE calculation does not increase the computational burden with respect to parameters selection (Duan et al., 2013).

Duan et al. (2013) introduced a normalized nonlinear definition for the TE in order to quantify the causal relationships. The normalized differential TE (NTE_{diff}) is defined as follows:

$$NTE_{x \rightarrow y}^c = \frac{2^{H^c(y_{i+h_1}|y_i^{k_1})} - 2^{H^c(y_{i+h_1}|y_i^{k_1}, x_i^{l_1})}}{2^{H_0} - 2^{H^c(y_{i+h_1}|y_i^{k_1}, x_i^{l_1})}} \in [0, 1] \quad (2.26)$$

where $H_0 = \log(y_{max} - y_{min})$ and y_{max} , y_{min} are the maximum and minimum values of y , respectively. $H^c(y_{i+h_1}|y_i^{k_1})$ and $H^c(y_{i+h_1}|y_i^{k_1}, x_i^{l_1})$ are the differential conditional entropies. The numerator term represents the information about y that is not explained by its own history but is explained by history of x . The denominator represents the information about y that is explained by the past of both x and y .

Similarly, the normalized differential DTE ($NDTE_{diff}$) is defined as

$$NDTE_{x \rightarrow y}^c = \frac{D_{x \rightarrow y}}{H^c(y_{i+h}|y_i^{k_1}) - H^c(y_{i+h}|y_i^{k_1}, z_{i+h-h_3}^{m_2}, x_{i+h-h_1}^{l_1})} \in [0, 1] \quad (2.27)$$

where $H^c(y_{i+h}|y_i^{k_1})$ and $H^c(y_{i+h}|y_i^{k_1}, z_{i+h-h_3}^{m_2}, x_{i+h-h_1}^{l_1})$ are the differential conditional entropies. $NDTE_{diff}$ represents the amount of information transferred from x to y via a direct pathway compared to the total amount of

information transferred to y from both x and z . (Duan et al., 2013)

The TE_{diff} and the DTE_{diff} can be approximated as follows :

$$T_{x \rightarrow y} = \frac{1}{N - h_1 - r + 1} \sum_{i=r}^{N-h_1} \log \frac{f(y_{i+h_1}|y_i^{k_1}, x_i^{l_1})}{f(y_{i+h_1}|y_i^{k_1})} \quad (2.28)$$

Where N is the number of samples and $r = \max\{(k_1 - 1)\tau_1 + 1, (l_1 - 1)\tau_1 + 1\}$.

Similarly, the DTE_{diff} can be approximated by:

$$DTE_{x \rightarrow y} = \frac{1}{N - h - j + 1} \sum_{i=j}^{N-h} \log \frac{f(y_{i+h}|y_i^k, z_{i+h-h_3}^{m_2}, x_{i+h-h_1}^{l_1})}{f(y_{i+h}|y_i^k, z_{i+h-h_3}^{m_2})} \quad (2.29)$$

where $j = \max\{(k_1 - 1)\tau_1 + 1, (k_2 - 1)\tau_3 + 1, -h + h_3 + (m_2 - 1)\tau_3 + 1, -h + h_1 + (l_1 - 1)\tau_1 + 1\}$. (Duan et al., 2013)

The conditional PDFs can be expressed by the joint PDFs which can be estimated by the Fukunaga method (Silverman, 1986) using a Gaussian kernel function. Considering q -dimensional vectors $[X_1, \dots, X_N]$ ($X_i \in \mathbb{R}^q$), the Kernel estimation for the q -dimensional vector $[x_1, \dots, x_q]^T$ is:

$$\hat{f}(x) = \frac{(\det \mathbf{S})^{-1/2}}{N\Gamma^q} \sum_{i=1}^N K\{\Gamma^{-2}(x - X_i)^T \mathbf{S}^{-1}(x - X_i)\} \quad (2.30)$$

where Γ is the bandwidth and is calculated from: $\Gamma = 1.06N^{-1/(4+q)}$. $\mathbf{S}$ is the covariance matrix of the data and K is the Gaussian kernel function:

$$K(u) = (2\pi)^{-q/2} e^{-\frac{1}{2}u} \quad (2.31)$$

Due to the high computational complexity of the kernel estimation of the joint PDFs, in particular for the DTE calculation, the selected embedding dimension should be limited. Alternatively, a large-scale system can be divided into small sub-systems and analyzed per each sub-system (Duan et al., 2013).

The statistical significance of the TE can be tested, for example, with the Monte Carlo method (Bauer et al., 2007a) or bootstrap method (Vakorin et al., 2009) using surrogate data.

The iterative amplitude adjusted Fourier transform (IAAFT) (Schreiber & Schmitz, 2000) method can be used to construct the surrogate data. According to Bauer et al. (2007a), a six sigma threshold for the significance level is an appropriate selection for a robust decision. Due to the difficulty of constructing surrogate data which satisfies the null hypothesis of the DTE surrogates, it

remains a challenge to determine a significance level for the DTE (Duan et al., 2013).

In comparison with the linear methods, the TE can be applied to more generalized cases which include nonlinear causal interactions. Therefore, the TE can provide a better estimation of causality in complex systems which are highly inter-connected (e.g., a system with numerous bidirectional interactions and recycle streams). On the other hand, the concept of the TE is similar to that of the GC except that the GC is framed in terms of prediction while the TE is framed in terms of uncertainty (Barnett et al., 2009). A possible advantage of the TE over GC is that TE depends solely on the estimation of multivariate entropies based on the PDFs, as such, fewer assumptions about the data are required than for GC (Bressler & Seth, 2011). Moreover, for Gaussian variables the two notions are equivalent (Barnett et al., 2009).

To conclude, TE is a model-free method which can be applied to both linear and nonlinear systems and is able to reveal causal relationships even when the time delay is inexplicit. However, the method is highly dependent on the estimation of PDFs. Thus, the computational burden increases significantly with the dimensionality of the analysis. Further research is required to establish more efficient and accurate PDF estimation (Duan et al., 2013). Moreover, determining the TE parameters such as prediction horizon and embedding dimension is a demanding task requiring a substantial computational effort. Finally, the TE requires that the series are WSS which is often not the case for industrial systems.

Nearest neighbors method

Similarly to the TE method, the nearest neighbors (NN) method is based on the concept of embedded vectors which provide a high dimensional representation of a dynamic system (Sauer et al., 1991). The NN method exploits the time delay and signal attenuation in order to provide a directionality measure (Bauer et al., 2005a).

Consider variable X with N samples. The embedded vector x_i for time instance i is defined as $x_i = [x_i, x_{i-k}, \dots, x_{i-(m-1)k}]$ where m is the embedding dimension and k is the time delay. All the embedded vectors of X can be arranged in the following matrix (Bauer et al., 2007b):

$$X = \begin{pmatrix} x_{(m-1)k+1} & \dots & x_1 \\ x_{(m-1)k+2} & \dots & x_2 \\ \vdots & & \vdots \\ x_N & \dots & x_{\tilde{N}} \end{pmatrix} \quad (2.32)$$

where $\tilde{N} = N - (m-1)k$ is the number of embedded vectors.

The K nearest neighbors of x_i are the embedded vectors that have the smallest Euclidean distance to x_i : $d_{i,j} = \|x_i - x_j\|$. The nearest neighbors of each x_i are denoted as $r_{i,j}$ where $j = 1, \dots, K$. Similarly, the nearest neighbors of each embedded vector y_i of Y are denoted as $s_{i,j}$ (Bauer et al., 2007b).

Every embedded vector x_i and y_i is assigned with a prediction value x_{i+h} and y_{i+h} , respectively, where h is the prediction horizon. The method evaluates how well the embedded vectors in X can predict the future values y_{i+h} and vice versa. For simplification, consider two time series X and Y , each with N variables and that $m = 4$ and $k = 1$. Assuming that the nearest neighbor of $x_4 = [x_4, x_3, x_2, x_1]$ is $x_{20} = [x_{20}, x_{19}, x_{18}, x_{17}]$. Then, if the distance between prediction values y_{4+h} and y_{20+h} is small, X can be considered as a good predictor of Y .

Accordingly, the mutual predictability from Y to X is defined as (Bauer et al., 2007b; Cecilio et al., 2016) :

$$D_i(X|Y) = \frac{1}{K} \sum_{j=1}^K |x_{i+h} - x_{s_{i,j}+h}| \quad (2.33)$$

where x_{i+h} is the prediction value of x_i while $x_{s_{i,j}+h}$ is the prediction value assigned according to the index of the j^{th} nearest neighbor of y_i .

The self-predictability of X is defined as :

$$D_i(X) = \frac{1}{K} \sum_{j=1}^K |x_{i+h} - x_{r_{i,j}+h}| \quad (2.34)$$

where x_{i+h} is the prediction values of x_i and $x_{r_{i,j}+h}$ is the prediction of the j^{th} nearest neighbor of x_i . The mutual and self-predictability are then scaled to give the following predictability improvement measure (Bauer et al., 2007b):

$$H(X|Y) = \frac{1}{\tilde{N}} \sum_{i=1}^{\tilde{N}} \frac{D_i(X|Y)}{D_i(X)} \quad (2.35)$$

Similarly, the complimentary predictability measure $H(Y|X)$ is calculated in order to assess the influence of X on Y . Finally, both measures are compared

in order to establish a directionality measure, $H_{x \rightarrow y}$:

$$H_{x \rightarrow y} = H(X|Y) - H(Y|X) \quad (2.36)$$

A positive value of $H_{x \rightarrow y}$ indicates on causality from X to Y while a negative value indicates causality from Y to X .

The statistical significance of the results can be determined using surrogate time series (Kantz & Schreiber, 1997; Theiler et al., 1992). Surrogate data methods preserve the power spectrum, auto-correlation function and probability density function of the original series except that their phase of frequency is randomized (Bauer et al., 2007b). For instance, the amplitude adjusted Fourier transfer (AAFT) method generates this type of series (Theiler et al., 1992). The main steps of the AAFT algorithm are as follows: (1) The data is rescaled according to Gaussian distribution. (2) The rescaled data is Fourier transformed and the phase of the surrogates is randomized. (3) The surrogates are scaled to the distribution of the original series by using an inverse Fourier transform. (Bauer et al., 2007b; Dolan & Spano, 2001)

Bauer et al. (2007b) suggest that 20 surrogates should provide satisfactory statistical results while keeping the computational level reasonable.

The null hypothesis is that X does not influence Y and is denoted as $\lambda_0 = H_{x \rightarrow y}$. The directionality measure is then calculated for each of the surrogate time series corresponding to X and Y : $\lambda_k = H_{x_{sur} \rightarrow y_{sur}}$, $k = 1, \dots, N_{sur}$. The null hypothesis can be rejected if λ_0 considerably differs from all other λ_k values obtained from all surrogates. This can be tested by comparing the mean value of all λ_k with λ_0 as follows (Bauer et al., 2007b):

$$\Omega_{X \rightarrow Y} = \frac{\lambda_0 - \mu_\lambda}{\sigma_\lambda} \quad (2.37)$$

where μ_λ and σ_λ are the mean and standard deviation of λ_k obtained from all the surrogate time series, respectively. According to Theiler et al. (1992), if

$\Omega_{X \rightarrow Y} \geq 3$, the null hypothesis can be rejected, i.e., X has influence on Y .

The parameters can be adjusted using guidelines provided by Bauer et al. (2005a, 2007b) based on several experimental studies. The number of nearest neighbors, K , has less impact on the directionality measure, however, it has to be at least equal to the number of cycles in the analyzed data in case of an oscillatory disturbance or the number of repetitive peaks in case of a non-oscillatory disturbance (Bauer et al., 2007b).

The procedure for selecting the parameters k , h , and m is as follows. First, the

embedding dimension is varied while k and h remain constant (typically set to $k = h = 1$). The m value for which the significance level reaches a maximum value is chosen. Next, the same procedure is repeated while k is varied and m is kept at its best value according to the previous step. Finally, the prediction horizon, h , is varied while m and k are kept at their optimal values according to the previous steps.

To sum up, the NN method offers a bivariate non-linear directionality measure for identifying the direction of propagation and root cause of a fault. The main advantage of the NN method lies in its straightforward and practical approach. In comparison with TE, it requires less computational effort since it does not require PDF estimation. Furthermore, less samples are needed to obtain consistent results. A drawback of the NN method is that it requires a careful selection of variables with similar time trends in order to produce useful results (Bauer et al., 2005a).

Causality estimator based on nonparametric multiplicative regression

The concept of nonparametric multiplicative regression (NPMR) originates from the field of ecology for habitat modeling and was introduced by McCune (2006, 2011). In that context, NPMR was used to find relationships between species occurrence and specific predictors such as environmental characteristics. The NPMR estimator aims to find causal relationships without estimating any coefficients in mathematical form. Instead, it tries to fit a local model to the data, e.g., local mean estimator or local linear regression (McCune, 2011). The contribution of each predictor to the model is defined by weighing the local observations near the target point via a kernel Gaussian function. Consequently, the weights of the observations diminish smoothly as their distance from the target point increases (McCune, 2011). The multiplicative nature of the NPMR estimator allows for interactions between the individual predictors. Ultimately, the NPMR-based estimator enables the identification of the predictors that have the greatest impact on each variable.

The NPMR-based estimator has several advantages compared with other causality estimators (Nicolau & Constandinou, 2016):

- It does not require any model estimation of specific form.
- It can be applied to both linear and nonlinear systems without any restriction on the order of the nonlinearity.
- It does not suffer from overfitting, a problem which the majority of nonlinear causality estimators suffer from. The overfitting is addressed in the estimator using leave-one-out cross validation.

- It can be applied both for bivariate and multivariate estimations without any modification.
- New observations can immediately be included in the estimation as soon as they become available.
- The statistical significance can be determined using surrogate data methods and the sensitivity measure Q can be used to evaluate the relative contribution of each predictor in the model.

Like GC, the NPMR-based estimator uses the past information of time series as predictors in order to establish causal relationships between variables. Consider a variable Y to be estimated : $Y = [y_1, y_2, \dots, y_N]$ and a matrix X with m predictors:

$$X = \begin{pmatrix} x_{1,1} & x_{1,2} & \dots & x_{1,m} \\ x_{2,1} & x_{2,2} & \dots & x_{2,m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N,1} & x_{N,2} & \dots & x_{N,m} \end{pmatrix} \quad (2.38)$$

A global response surface of Y is built from its m predictors using a multiplicative kernel smoother (McCune, 2006). This is achieved by estimating each y_n from its local neighborhood in the predictor space $X_n = [x_{n,1}, x_{n,2}, \dots, x_{n,m}]$ (Nicolaou & Constandinou, 2016). The influence of each predictor is defined by its corresponding tolerance of the kernel smoother $\sigma_j (j = 1, \dots, m)$, which is a unique feature of NPMR (McCune, 2006; Nicolaou & Constandinou, 2016).

Throughout this study, the local neighborhood is defined as a weighted mean and the weights are estimated using a Gaussian kernel smoother.

$$w_{i,j} = e^{-\frac{1}{2}[(x_{i,j} - x_{n,j})/\sigma_j]^2} \quad (2.39)$$

The weights represent the distances of each predictor from the target point (n) estimated with a Gaussian kernel weighting function with a tolerance (standard deviation, σ_j) (Nicolaou & Constandinou, 2016). The Gaussian tolerance defines how rapidly the weights subside with distance from the target point. Namely, selecting a large standard deviation corresponds to taking a broad local neighborhood in the predictor space in order to estimate a target point and vice versa. (McCune, 2006; Nicolaou & Constandinou, 2016)

Consequently, the estimation of a target point y_n is defined as :

$$\hat{y}_n = \frac{\sum_{i=1, i \neq n}^N y_i (\prod_{j=1}^m w_{i,j})}{\sum_{i=1, i \neq n}^N (\prod_{j=1}^m w_{i,j})} \quad (2.40)$$

By omitting the target point n from the estimation, overfitting is avoided and error estimates become more realistic (McCune, 2006).

The basic idea of NPMR can be used in the context of causality analysis by extending the predictor space to include past information. This is obtained by using time-delayed embedded vectors as predictors. Consider embedded vector $\tilde{x}_n = [x_n, x_{n-\tau}, \dots, x_{n-(d-1)\tau}]$ where d is the embedded dimension and τ is the time delay. The NPMR-based causality estimator can be applied to estimate Y using only its own time-delayed equivalent $\tilde{Y}$ or combining both time-delayed predictor variables, $\tilde{X}$ and $\tilde{Y}$. Similarly to GC, causal relationships can be established by calculating the error variances of the predictions. In case of a bivariate estimate, the NPMR-based causality is defined as follows (Nicolau & Constandinou, 2016):

$$C_{NPMR}(X_j \rightarrow Y) = \log\left(\frac{\sigma_{(Y, \tilde{Y})}^2}{\sigma_{(Y, (\tilde{Y}, \tilde{X}_j))}^2}\right) \quad (2.41)$$

where X_j is the j^{th} predictor and $\sigma_{(Y, \tilde{Y})}^2$, $\sigma_{(Y, (\tilde{Y}, \tilde{X}_j))}^2$ are the error variances when past values of Y are used as predictors and when both past values of Y and X_j are used as predictors, respectively. This definition can be extended to conditional / multivariate causality estimation which follows the standard conditional GC (Nicolau & Constandinou, 2016):

$$C_{NPMR}(X_j \rightarrow Y/Z) = \log\left(\frac{\sigma_{(Y, \tilde{Y}, Z)}^2}{\sigma_{(Y, (\tilde{Y}, \tilde{X}_j, Z))}^2}\right) \quad (2.42)$$

where Z corresponds to all the predictor variables to be included in the estimation excluding X_j . The above definitions of C_{NPMR} are not bounded, meaning that negative values can be obtained. Negative values simply imply that there is no causal dependency between the time series.

The relative contribution of each predictor, can be evaluated with sensitivity analysis where each predictor j is nudged by a small proportion and the resulting change in the prediction is measured as follows:

$$Q(Y/X_j) = \frac{\sum_{i=1}^N |\hat{y}_i^+ - \hat{y}_i| + |\hat{y}_i^- - \hat{y}_i|}{2N|y_{max} - y_{min}|\Delta} \quad (2.43)$$

where y_{max} and y_{min} are the maximum and minimum values of Y , respectively. $\hat{y}_i$ is the estimated value of y_i . $\hat{y}_i^+$ and $\hat{y}_i^-$ are the estimated response when nudging X_j up and down, respectively and Δ is a small proportion by which each predictor

is nudged (Nicolaou & Constandinou, 2016). All the estimations are calculated without cross-validation (i.e., by including $i = n$ in Eq. 2.40). High values of Q indicate a high sensitivity of the response variable to a particular predictor.

The overall model fit can be estimated via "cross R^2 " according to the relationship between the residual sum of squares (RSS) and the total sum of squares (TSS) (McCune, 2011):

$$\chi R^2 = 1 - \frac{RSS}{TSS} = 1 - \frac{\sum_{i=1}^N (y_i - \hat{y}_i)^2}{\sum_{i=1}^N (y_i - \bar{y}_i)^2} \quad (2.44)$$

where y_i is the predicted variable, $\hat{y}_i$ is the estimated variable and $\bar{y}_i$ is the mean of the predicted variable. A χR^2 value close to 1 indicates on a good model fit (Nicolaou & Constandinou, 2016).

The statistical significance of C_{NPMR} can be evaluated using surrogate data. For instance, the AAF_T method (Theiler et al., 1992) can be used to generate surrogate data. The number of surrogates for a particular statistical level can be determined via $N_{sur} = \frac{1}{\alpha} - 1$ where α is the desired statistical level. The significance level is set to the maximum values of C_{NPMR} obtained from all surrogate estimates (Nicolaou & Constandinou, 2016).

Selecting an appropriate time delay is essential for taking into account longer dynamics (Nicolaou & Constandinou, 2016). Different methods are available for estimating the time delay. For instance, the selection can be based on the minimum mutual information (Fraser & Swinney, 1986) or the auto-correlation function (Nicolaou & Constandinou, 2016). Although it is necessary to select an appropriate embedding dimension, the selection should not affect the pattern of causality but rather its amplitude (Nicolaou & Constandinou, 2016). Cao (1997) proposed a practical approach for estimating the embedding dimension. Alternatively, a threshold for the embedding dimension can be selected according to the model fit (Eq. 2.44) improvement when increasing the embedding dimension. Finally, the kernel tolerance can be tuned via an iterative procedure or it can be estimated from the data itself. The NPMR-based estimator allows for each predictor to have a different tolerance factor, i.e., the influence of each predictor on the estimation can be adjusted (McCune, 2011; Nicolaou & Constandinou, 2016).

To conclude, the NPMR-based estimator quantifies cause and effect relationships between a response variable and its predictor variables. The estimator addresses many of the limitations of other causality estimators. Its nonparametric nature and its ability to capture causality in nonlinear and multivariate systems make

it appealing for industrial applications.

2.3.3 Other methods and summary

In addition to the methods described above, several other methods are reported in literature for capturing causality between time series. For example, Bayesian nets (Cowell et al., 1999) provide a causal probabilistic graph where nodes denote faults or process variables and arcs denote conditional probabilities. Its major limitation is that it has to be a directed cyclic graph which is not suitable for dynamic processes with cycles that are very common (Yang & Xiao, 2012). However, a cyclic algorithm has been developed to address this limitation (Richardson & Sprites, 2001). In addition, the physical explanation of probabilities is not straightforward and data requirements to build the model are hard to meet (Yang & Xiao, 2012).

Yang & Xiao (2006) proposed to use a probabilistic signed directed graph (PSDG) in order to describe the propagation of faults within variables. PSDG can be treated as a special case of a Bayesian network, hence, Bayesian inference can be used to estimate the probabilities. In this case, the conditional probabilities of faulty events are taken into account to describe causes and effects among variables with respect to the fault probability. Unlike Bayesian nets, PSDG requires special treatment of cycles (Yang & Xiao, 2006). The main limitation of PSDG is the computational complexity involved in building the model. Moreover, obtaining the conditional probabilities is not straightforward since real equipment usually does not allow designed fault experiments so often they are estimated from experiences (Yang & Xiao, 2006).

Faes et al. (2008b); Lungarella et al. (2007) and Smith et al. (2011) summarized and compared different methods for capturing causality in bivariate and multivariate environments, respectively. Together, these studies indicate that no method alone is powerful enough to replace the others and they complement each other (Yang & Xiao, 2012; Yang et al., 2014). The majority of the data-based methods fail to capture direct causality since they are pairwise (Yang & Xiao, 2012). For instance, if two variables are driven by a third variable, one might still find spurious causality between these two variables. Thus, in real applications, one should try several methods to obtain reasonable results. Alternatively, process knowledge can be used to validate the results of the data-based analysis. (Yang & Xiao, 2012)

Each of the data-based methods has its own advantages and limitations, therefore

it is difficult to recommend a single method for a specific application. Several aspects should be considered when selecting a certain method, e.g., nonlinearity of the system, computational burden and the system complexity (i.e., existence of bidirectional / recycle streams). For instance, for systems with a simple topology, straightforward pairwise analysis such as GC or cross-correlation might be sufficient to get useful results. However, for a large-scale system with a high-level of connectivity, multivariate analysis should be considered.

The preeminent challenge in data-based causal analysis is establishing true direct causality relationships. It seems, therefore, that a fusion of different methods is vital to obtain reliable results. In real applications, one method can be tried at first, and then additional methods can be used for validation or comparison (Yang & Xiao, 2012). Alternatively, process insights from process schematic or site experts can be used to validate the results of the data-based analysis (Bauer et al., 2005b; Yang & Xiao, 2012).

2.4 Combining data-based and topology-based models

Process knowledge and data are both means of capturing causality in chemical processes. However, neither of them is sufficient for industrial applications due to redundancy and errors in the resulting models (Yang et al., 2014). Moreover, recent studies (Bauer et al., 2005b; Yang et al., 2012) highlight the need to utilize process insights derived from process schematic or site expertise in order to validate the results of the data-based analysis and vice versa. Consequently, in recent years there have been several attempts to combine data-based analysis with topology-based models for validation purposes. For instance, an SDG is typically constructed from process knowledge derived from P&ID. However, the main problem of such causal models is the lack of quantitative information to confirm its reliability (Yang et al., 2014). Thus, the resulting SDG should be validated by process data before being used for industrial applications. In their comprehensive study, Yang et al. (2010b, 2012) applied both the cross correlation method and TE in order to validate an SDG constructed from process knowledge. Using both methods, arcs in the SDG can be validated one by one, hence, the computational effort is proportional to the number of arcs. Given a validated SDG, it can be used for fault propagation and root cause analysis (Yang et al., 2012).

In some cases, process data is readily available while process knowledge is limited. In these cases, process knowledge can be used to validate a data-driven causal

model. One possibility is to check for reachability between two variables by searching for consistent paths (Yang et al., 2012). Accordingly, Jiang et al. (2008) introduced the concept of a control loop digraph and utilized the adjacency matrix for diagnosis of the root cause of plant-wide oscillations. A unique property of an adjacency matrix, X , is that the $(i, j)^{th}$ element of X^k gives the number of k step sequences from i to j (Jiang et al., 2008). If each non-zero element in each X^k matrix is replaced with '1', then, for a digraph with N nodes and adjacency matrix X , the reachability matrix R is defined as follows (Mah, 1989) :

$$R = (X + X^2 + X^3 + \dots + X^N) \quad (2.45)$$

The $(i, j)^{th}$ element of R indicates whether there exists any pathway from node i to node j in a digraph. As an example, consider the digraph and its corresponding adjacency matrix in Fig. 2.3. The element (2,5) of matrix X^2 shows that there are two 2-step sequences from b do d ($b \rightarrow c \rightarrow e$ and $b \rightarrow d \rightarrow e$). In addition, matrix R shows that node a can reach all other nodes, but cannot be reached by any other node.

$$X^2 = \begin{bmatrix} 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad R = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Figure 2.3. A digraph and its adjacency, X^2 and reachability matrices (Jiang et al., 2008)

Based on the concept of adjacency and reachability matrices, Jiang et al. (2008) proposed a method for detecting the source of an oscillatory disturbance by searching for nodes in a control loop digraph which can reach all the other oscillatory variables. This method can be combined with other data-based methods in order to provide a complete procedure for detection and diagnosis of

plant-wide disturbances.

Moreover, several attempts have been made to develop an automated tool for the detection and diagnosis of plant-wide disturbances by combining data-based analysis with process topology information. Yim et al. (2006) designed software which given an electronic P&ID and results from a data-based analysis, allows the user to perform queries about the plant and detect the root cause of disturbances. This hybrid scheme combines the plant topology information derived from an XML description of the process according to the CAEX schema and a data-based analysis tool called plant-wide disturbance analysis (PDA). The methods in the prototype software include: path (physical and control) finding between two specified points, analysis of control loops and indicators and root cause analysis. Furthermore, Thambirajah et al. (2009) introduced a cause-and-effect analyzer which combines a data-based analysis with the process connectivity information derived from an XML description of a process schematic. In their work, Thambirajah et al. (2009) used a CAEX description of the process schematic in order to generate a connectivity matrix representing the process topology. Then, the cause-and-effect analyzer identifies candidates for the root cause of disturbances based on a data-driven causality matrix. A search through the connectivity matrix by a search algorithm determines whether a physical propagation path is feasible between the postulated root causes and all the affected variables and which is the most probable root cause and propagation path (Thambirajah et al., 2007, 2009). The search algorithm uses a DFS (Cormen et al., 2001) which starts at a specified node and searches along a set of nodes until it reaches a certain termination criteria, at which point it backtracks and continues to search. The cause-and-effect analyzer searches through the connectivity matrix representing a schematic of a chemical process to find paths by which disturbances can propagate through the process. Thereby, a causal model derived from process measurements can be validated and the postulated root cause of a disturbance can be verified. (Thambirajah et al., 2009)

To conclude, this chapter presented the concepts of causality and connectivity and the differences among them. The main methods for capturing causality from process data and from process knowledge were described and evaluated according to their characteristics. Finally, several existing techniques for combining data-based and topology-based models were presented. Next chapter presents four methodologies for hybrid causal analysis by combining a topology-based model with both linear and nonlinear data-based estimators. The hybrid causal

analysis was developed using a DFS search algorithm which is based upon the cause-and-effect analyzer introduced by Thambirajah et al. (2009) and the concept of control loop digraph (Jiang et al., 2008) which were discussed earlier in this chapter.

3. Causal analysis by combining data-based methods with process connectivity information

In this chapter, the hybrid approach for combining data-based causal analysis with connectivity information is explained in detail, in particular, the search algorithm and its logic for finding direct and indirect pathways. Based on this approach, four methodologies for causal analysis have been developed based on several linear and nonlinear causality estimators.

3.1 The hybrid causal analysis

The studies presented thus far (Thambirajah et al., 2007, 2009; Yim et al., 2006) highlight the need to combine the information on the physical connectivity of a process with data-based causal analysis. These studies focus on searching for feasible propagation paths between process elements for validating the results of a data-based causal analysis or for root cause analysis. However, when investigating highly inter-connected systems with numerous bidirectional and recycle streams, finding feasible propagation paths among process components might not be sufficient to eliminate all the spurious results from the data-based analysis.

This study proposes a new approach for incorporating the connectivity information into a data-based causal analysis. The connectivity information is integrated into the data-based analysis via a unique search algorithm whilst the prime aim is to reduce the number of spurious results and at the same time minimize the computational effort throughout the analysis. The outcome of the analysis is an enhanced causal model depicting the fault propagation path.

When a fault propagates through a system it may stop due to signal attenuation (Yang et al., 2010a). Data-based methods capture the process causality based on the level of the interactions in the system. Therefore, while topology-based models capture the entire physical connectivity in a system, data-based methods

capture only the causal interactions associated with a fault. Hence, the proposed hybrid causal analysis takes into account only the connectivity information which is associated with the faulty variables.

The causal analysis aims to retrace the propagation path of a disturbance via control loops. The cornerstone of the causal analysis is the search algorithm which has two main functionalities: (1) finding all feasible propagation paths between two controllers. (2) checking if a path is direct or indirect. Explicitly, the search algorithm searches through the connectivity matrix extracted from the P&ID diagram of the process in order to find direct pathways between two controllers. If there is no direct physical path from one controller to another, it can be assumed that there is no causal dependency between them. The ability of the search algorithm to determine whether a physical path between two controllers is direct or indirect facilitates the analysis and reduces the results of the data-based causal analysis which do not represent direct causality. Furthermore, this type of hybrid analysis allows tackling systems with a high-level of connectivity while simultaneously minimizing the computational burden.

Figure 3.1. The overall approach for hybrid causal analysis

Fig. 3.1 presents a general scheme of the overall approach for the hybrid causal analysis: first, a topology-based model in the form of a connectivity matrix is extracted from the XML scheme of the process using AutoCAD P&ID. Then, once a fault is detected, data-based causal analysis is implemented in conjunction with

the process connectivity information by the virtue of the search algorithm. Several data-based methods are available for estimating the causality as presented in Fig. 2.2. This thesis uses four methodologies for causal analysis based on the following estimators: GC, TE, NN and NPMR-based causality estimator. The methodologies have been developed by taking into account the specific characteristics of each causality estimator. The outcome of the analysis is a causality matrix which contains the structural information for constructing the causal model depicting the propagation path and the root cause of a fault. A detailed description of the search algorithm and its logic for finding direct paths between control loops are given below.

3.2 The search algorithm

The developed search algorithm is based on a graph traversal which allows one to search through a series of nodes ensuring that each node is traversed only once (Thambirajah et al., 2007). In particular, this technique uses a DFS algorithm (Cormen et al., 2001) which begins to search from a specified node and continues through series of nodes until it reaches a termination, at which point it backtracks and continues searching (Thambirajah et al., 2009).

In this case, the algorithm searches through the connectivity matrix to find pathways between two control elements, typically, indicators since these are the measurement points. The recursive algorithm starts by moving from the row of the 'source' variable and searches in the connectivity matrix for '1' which indicates a direct connection between the row and column elements. The search proceeds to the row of the column element and so on until it reaches one of the following termination conditions: (I) it reaches the 'target' variable and hereby the path is found, (II) it reaches a component which had been visited before or (III) it reaches a component which is not connected to any other component (i.e., its row is empty). The algorithm then backtracks to follow all other pathways with the same termination conditions (Thambirajah et al., 2009). Consider the connectivity matrix in Fig. 3.2 as a generic example for a search for paths starting from Element-006 towards Element-001 (Thambirajah et al., 2009). Element-006 is connected to Element-005 which is connected to Element-007. Element-007 is connected to the target Element-001, hence the search reaches a termination condition and the path is found. The algorithm then backtracks to Element-004 which is not connected to any element, thus, the search ends.

More illustrative examples for the search algorithm implementation can be found in (Thambirajah et al., 2007, 2009) and a Prolog code of the algorithm can be

Figure 3.2. An example of depth-first search algorithm used to find paths from Element-006 to Element-001 (Thambirajah et al., 2009)

found in (Yim et al., 2006).

3.2.1 The search for a direct path

Once the search algorithm finds all physical pathways between a 'source' and 'target' variables (in this case, control elements), the algorithm checks every pathway and determines whether it is direct or indirect. According to Jiang et al. (2008), a direct path from controller i to controller j exists if the output of controller i directly affects the output of controller j without any intermediate effect on any other controller. Based on this concept, the algorithm searches for a direct path between two control elements. The algorithm checks every physical pathway originating from a 'source' controller i to a 'target' controller j and checks if the path traverses a control element which belongs to a controller that is neither i or j . Specifically, a path between controllers i and j is considered direct if it is comprised only of equipment / piping elements and / or control elements which belong only to the 'target' controller j .

In the initial phase, all the components in the connectivity matrix are classified into four types: equipment (including pipelines), controllers, sensors and valves. Then, the algorithm checks the type of each element in a path. If it finds a control element (valve, sensor or controller) which does not belong to the 'source' or 'target' variables, the corresponding path is indirect. Otherwise, if the path does not traverse the 'source' controller, it is considered as direct. The logic of this algorithm is illustrated in Fig. 3.3.

As an example, consider a search for a direct path from controller PC-651 to

Figure 3.3. The logic of finding a direct path between two controllers (publication I)

PC-652 using the connectivity matrix in Table 3.1. The corresponding output of the algorithm is shown in Fig. 3.4. First, the algorithm specifies the 'source' and 'target' points which are the pressure indicators PI-651 and PI-652, respectively. Next, the algorithm starts by identifying that PI-651 is connected to SG1 steam line (denoted by '1' in the first column of the connectivity matrix) which has two paths leading to PI-652. However, only path 2 is considered as direct since it is comprised only of equipment elements while path 1 traverses through the 'source' controller 'PC651' and therefore it is not considered as direct.

Table 3.1. An example of a connectivity matrix ('PV' denotes a control valve,'PC' denotes a pressure controller, 'PI' denotes a pressure indicator and 'SG' denotes a group of steam cylinders) (publication I)

Element	PI-651	SG1_Steam_Line	PC-651	PV-651	SG-1	PI-652
PI-651	-	0	1	0	0	0
SG1_Steam_Line	1	-	0	0	1	0
PC-651	0	0	-	1	0	0
PV-651	0	0	0	-	1	0
SG-1	0	0	0	0	-	1
PI-652	0	0	0	0	0	-


```

Checking cause and effect relationship between PI-651 and PI-652...
PI-651 is connected to
SG1_Steam_Line
There are 2 feasible propagation paths from
SG1_Steam_Line to PI-652...

Path 1 is                Path 2 is
SG1_Steam_Line           SG1_Steam_Line
PI-651                   SG-1
PC-651                   PI-652
PV-651
SG-1
PI-652

There is a direct link between SG1_Steam_Line and PI-652...

The direct path is:
SG1_Steam_Line
SG-1
PI-652

```

Figure 3.4. Example 1: The output of the search algorithm (publication I)

3.3 Integrating the connectivity information with the causality estimators

Four causal methodologies have been developed throughout this study based on the following causality estimators: GC, TE, NN and NPMR-based estimator. Each methodology has been developed by considering the specific characteristics of each estimator, particularly whether it is bivariate or multivariate.

Granger causality

In the case of GC, in this study the conditional GC (Guo et al., 2008) is implemented as a single step MV analysis by estimating MVAR models for all the variables. Consequently, the connectivity information is used in order to exclude spurious results from the GC causality matrix as an additional step. The refinement procedure of causality matrix X is performed as follows (publication I):

1. Select the next non-zero element (i, j) in causality matrix X that has not been validated.
2. Check whether there is a direct path from controller i to controller j using the search algorithm. The search for a direct path is done according to Section 3.2.1: the algorithm first finds all physical pathways between controllers i and j and then checks whether any of them is direct. If it finds at least one direct path, the causality between controller i to j is confirmed.
3. If there is no direct path from controller i to controller j , $X(i, j) = 0$.

4. Repeat steps 1-3 until all non-zero elements in the causality matrix are checked.

Transfer entropy and nearest neighbors

The TE and NN, on the other hand, are implemented in two phases: first a bivariate analysis is performed followed by a multivariate analysis which aims to exclude redundant results from the bivariate analysis. Accordingly, the connectivity information is integrated in two phases. Fig. 3.5 illustrates the proposed methodology for implementing TE.

Figure 3.5. The two-phase methodology for implementing TE (publication II)

In phase I, the search algorithm finds all physical pathways between each controller i and j . If there is no physical pathway from controller i to j , it can be concluded that there is no causal pathway as well. Otherwise, the search algorithm checks if there is a direct path between these controllers. If there is a direct path, the TE from controller i to j is calculated. In phase II, all the indirect / spurious interactions which were obtained in phase I are evaluated by calculating the DTE. In this phase, the search algorithm is utilized in order to obtain the intermediate controllers of each indirect path using the connectivity matrix. When dealing with small-scale systems, obtaining the indirect paths is a straightforward task which can be achieved manually. However, in large-scale or complex systems with numerous pathways and recycle streams, obtaining all the indirect pathways manually can be an extremely strenuous and time consuming task. The ability to utilize the search algorithm to obtain indirect pathways makes the analysis notably faster and efficient. Once all the indirect paths are obtained by the search algorithm, the DTE is calculated for each path in order to determine whether the causality can be considered as direct. The logic

of calculating the TE / DTE in each phase is illustrated in Fig. 3.6.

Figure 3.6. The procedure for calculating the TE based on the process connectivity: Phase I (left) and Phase II (right). TE=Transfer Entropy, NTE=Normalized Transfer Entropy, DTE=Direct Transfer Entropy, NDTE=Normalized Direct Transfer Entropy (publication II)

A similar methodology was developed for the NN method: a two-phase analysis wherein bivariate estimation is calculated in phase I and multivariate estimation is calculated in phase II as a tool for discriminating between direct and indirect connectivity. The implementation of phase I is similar to the TE implementation: the search algorithm finds direct pathways based on the connectivity matrix of the process and the bivariate NN directionality measure is calculated for each direct path. However, in phase II, the indirect pathways are obtained according to a new connectivity matrix which is based on the initial causality matrix. Namely, each '1' in the new connectivity matrix corresponds to a positive directionality measure calculated in phase I. Then, in phase II, a new multivariate directionality measure (publication III) is used to evaluate each indirect path based on the new connectivity matrix. The proposed MV directionality measure takes into account the effect of variable Y on X via n intermediate variables Z according to the

following formula:

$$H(X|Y, Z) = \frac{1}{\tilde{N}} \sum_{i=1}^{\tilde{N}} \frac{D_i(X|Y)}{D_i(X) + \sum_{j=1}^n D_i(X|Z_j)} \quad (3.1)$$

where $D_i(X|Z_j)$ is the mutual predictability from intermediate Z_j to X and n is the total number of intermediate variables. The nominator can be seen as the directionality measure from Y to X which is scaled by the denominator representing the self-directionality of X and the sum of the directionality measures from each Z_j to X . Then, analogously to Eq. 2.36, a direct causality from X to Y can be established according to the following equation:

$$H_{x \rightarrow y, z} = H(X|Y, Z) - H(Y|X, Z) \quad (3.2)$$

A value of $H_{x \rightarrow y, z}$ that is considerably higher than zero, can be taken as evidence for direct causality from x to y . The estimated parameters (m, k, h) remain the same as in the bivariate analysis. Several examples demonstrating the application of the proposed MV directionality measure on simulated data can be found in publication III.

Figure 3.7. The proposed methodology for causal analysis based on nearest neighbors method (publication III)

A scheme of the methodology for causal analysis based on the NN method is shown in Fig. 3.7. In addition, the explicit logic of calculating the directionality measure between each pair of controllers (i, j) in each phase is presented in Fig. 3.8.

In phase I, similarly to the TE implementation, the bivariate NN directionality

Figure 3.8. The logic of calculating the nearest neighbors directionality measure in phases I & II

measure is calculated only for the paths which are considered as direct according to the process topology. The initial causality matrix contains only positive directionality values corresponding to paths which are considered as direct by the search algorithm and zeros indicating either a lack of physical connectivity between the controllers or a pathway that is indirect. Then, as an intermediate step, a new connectivity matrix is constructed according to the initial causality matrix by setting each non-zero element in the causality matrix to '1' in the new connectivity matrix. In phase II, the new connectivity matrix is utilized in order to find all possible propagation paths between each (i, j) pair of controllers whose directionality been calculated in phase I. For each indirect path, the newly proposed multivariate directionality measure (Eq. 3.2) is calculated. Ultimately, if the mean value of all the indirect paths for each pair is considerably higher than zero (>0.1), a direct causality can be inferred.

NPMR-based causality estimator

The methodology for implementing the NPMR-based causality estimator follows a similar logic as the TE and NN implementation. This is primarily due to the

fact that all three methods are implemented both as bivariate and multivariate analysis in this study. However, unlike the TE and NN, the NPMR-based causality analysis is implemented in a single phase (see Fig. 3.9). In addition, all the estimations undergo a statistical evaluation using surrogate data which further contributes to the reliability of resulting model.

Figure 3.9. The methodology for causal analysis based on NPMR-based estimator (publication IV)

First, the search algorithm searches for all propagation paths between any (i, j) pair of controllers. If there is no path, the algorithm continues to the next pair, thus, no calculation is needed for controllers which have no feasible propagation path connecting them. Then, the search algorithm checks if there is a direct path between the controllers. If there is a direct path, the bivariate NPMR-based causality is calculated and the estimated value undergoes a statistical evaluation. Otherwise, the conditional (MV) NPMR-based causality is calculated for all the indirect paths and the maximum value is taken for statistical evaluation. The logic of the NPMR-based analysis is illustrated in Fig. 3.10.

Figure 3.10. The logic of the NPMR-based causality analysis (publication IV)

To sum up, four methodologies for hybrid causal analysis were developed based on different linear and nonlinear causality estimators. A unique search is utilized in order to integrate the connectivity information with the data-based analysis. The fundamental logic behind the majority of the developed methodologies is to estimate the causality based on the physical directionality between two controllers. First, the search algorithm is utilized in order to find direct and indirect propagation paths between two control loops using the connectivity matrix. Then, the causality can be estimated based on the identified propagation paths: if there is no feasible propagation path between two controllers, the causality is not estimated, if a direct path exists, bivariate causality is estimated while MV causality is estimated for indirect paths in order to exclude redundant links from the resulting model. This automated procedure facilitates the analysis and produces an enhanced causal model with less spurious results.

4. Description of the board machine and the case study

In this chapter a description of the industrial board machine and its control strategy is provided, in particular its drying section. Then, a detailed description of the process case study involving valve stiction in the drying section is given including the procedure of variable subset selection.

4.1 General description of the board making process

The case study of this thesis involves a paperboard machine (BM) located in Stora Enso's Kaukopää mills in Imatra, Finland. The BM produces three-layer liquid packaging boards and paper cups. A schematic description of the board making process is shown in Fig 4.1.

The process begins with the preparations of the raw materials in the stock preparation section. Different types of pulp are refined and blended according to a specific recipe in order to achieve the desired board properties (Jämsä-Jounela et al., 2013). In addition, several additives and chemicals are added to improve the quality of the board. Since the BM produces a three-layer board, there are three separate preparation sections for each layer of the board. The blended stock is then transferred to the approach flow system (short circulation). First, the stock is diluted in the wire pit to the correct consistency and then it is cleaned in the hydro-cyclone cleaning plant in order to remove impurities (Tikkala, 2014).

Then, the stock moves to the headbox, from where it is sprayed evenly over a wire to form a solid web (Norman, 2000).

Next, the board is dried in several stages. First one is the wire section where the water is drained through the wire. In addition, the webs are combined to form the final structure of the product. The second stage is the press section where the web is pressed between rollers to remove water. Finally, the remaining water is evaporated in the drying section by steam filled drying cylinders. After drying, the board is calendered in two phases to achieve the desired surface properties

Figure 4.1. Overview of the board making process (Tikkala, 2014)

such as gloss, smoothness, density and thickness. Lastly, the board is reeled and transferred to post processing (Tikkala, 2014).

4.2 The control strategy of the board machine

The BM is controlled by two main systems: a distributed control system (DCS) and a quality control system (QCS). The QCS system aims to control the quality variables whereas the DCS system is in charge on the basic control level (Tikkala, 2014). The QCS uses Honeywell's Robust Model-Predictive Control Technology (RMPCT) to control the main quality variables: basis weight, moisture and thickness which are measured after the calender section (Tikkala, 2014). The set-points of the quality variables are delivered to the lower level controllers by the DCS system.

The QCS system operates in two dimensions in order to control the web quality: machine direction and cross direction. In the machine direction, the quality variables are controlled by providing set-points to the lower level controllers. The

basis weight control is achieved by regulating the stock flow controller set-points and the moisture is controlled by providing set-points to the steam pressure controllers in the drying section. In the cross direction, the basis weight is controlled by the dilution water in the middle layer headbox and the moisture is controlled with a steam box located before the press section and a moisturizing device in the drying section. The thickness is controlled at the second calender (Tikkala, 2014).

The DCS level consists of approximately 500 controllers that adjust the flows, pressure, level, etc., in the BM. The main control loops in the DCS level, the stock flow and the steam pressure controllers are stabilizing controllers that receive their set-points from the QCS system. The stock flow controllers are located in the approach flow system. The stock flow is controlled by adjusting the rotation speed of the pumps in each approach flow system. There are three separate controllers adjusting the rotational speed according to the desired layers ratio. The steam pressure controllers are located in the drying section (Tikkala, 2014).

4.3 The drying section

In the drying section the remains of the excess water are evaporated to achieve the desired moisture content in the board. The web is heated by steam filled cylinders and the latent heat released from the condensate is used to evaporate the bound water (Kuuluvainen, 2012). The cylinders are located under a hood which is ventilated in order to remove moisture. In addition, heated air is blown into drying pockets between the cylinders to facilitate moisture removal.

The condensate from the cylinders is collected by siphons to tanks where the steam and condensate are separated. Steam is then recycled back to the process whereas the condensate is returned to a power plant.

The drying section is divided into six steam groups (SGs) containing in total 74 drying cylinders. Each SG and its corresponding condensate tank form a drying group (DG). Each DG has its own controllers that adjust the steam pressure, the steam pressure difference between steam and condensate headers and the level of the condensate tanks. The tension of the drying fabric is controlled separately in each drying group by hydraulic actuators in order to provide adequate support to the web. A scheme of the drying section and its controllers is presented in Fig. 4.2. PC660 (located in SG8) is the steam pressure controller which receives its set-point from the QCS system. The cylinder on the upper left corner of

Fig. 4.2 is used to collect the steam from the process which is then condensed and transferred to C1. The condensate is then delivered to C2 from where it is collected and returned to a power plant.

Figure 4.2. The drying section of the BM. Red pipelines denote steam, purple pipelines denote a mixture of condensate and steam, and blue pipelines denote condensate. SG=Steam Group, PC=Pressure Controller, C=Condensate Tank, LC=Level Controller, PI=Pressure Indicator. The drying section includes six DGs: each DG consists of a single SG and its corresponding condensate tank and their controllers, e.g., SG1, C2 and the controllers PC651, PC652, PC1653 and LC651 comprise DG1 (publication I)

The steam pressure is controlled by two steam headers: 5 and 10 bar headers (denoted by the two red lines at the top of Fig. 4.2). PC668 provides 10 bar steam to the system and pressure indicator PI667 is connected to the 5 bar steam header. SG1 uses only 5 bar steam while the steam pressure of the other groups is controlled by two valves connected to each steam header, depending on the pressure demand. If the pressure demand is low, only 5 bar steam is used, whereas if higher pressure is needed, 10 bar steam is used as well.

The pressure difference control is important for proper operation of the drying section: it has to be high enough to enable efficient condensate removal by the siphons and simultaneously low enough to avoid blowing steam directly through the cylinders. This is achieved by manipulating two control valves in the steam outlet of each condensate tank. The level of each condensate tank is controlled by adjusting the outlet flow. Fig. 4.3 presents a scheme of the control system of a single DG.

Figure 4.3. Control of the steam and condensate system for a single drying group (PC=Pressure Controller, PDC= Pressure Difference Controller, LC= Level Controller)

4.4 The process case study

The case study is focused on the drying section of the BM since the web conditions such as the temperature and moisture content have a substantial effect on the board quality, therefore, they require proper control and monitoring (Karlsson, 2000). The drying section is subjected to many types of faults associated with valves, e.g., clogging, stiction, jamming and leakages. Due to the high connectivity between the controllers in the drying section, faults can easily propagate through the process units. Causal analysis in this section enables to reveal the causal dependencies between the control loops and disclose the root cause of a fault.

The present case study involves valve stiction in the pressure controller PC1652 of SG3. Valve stiction is one of the most dominant faults in the drying section and has a detrimental effect on the board quality and the control performance (Pozo Garcia et al., 2013). The cyclic nature of stiction manifests as an oscillatory behavior of the control loops since the stiction delays the valve's movement while the process input remain the same. Oscillation caused by valve stiction can easily propagate via the control loops and eventually degenerate the overall control performance (Pozo Garcia et al., 2013). The stiction in PC1652 was initially diagnosed using the stiction detection system proposed by Zakharov et al. (2013) and was subsequently confirmed based on the long-term maintenance records of the plant. Fig. 4.4 presents the normalized time series of the controlled variables of the plant.

(PVs) where the signal of PC1652 is colored in red. The sampling period is 10s and the series were normalized by removing the mean and scaling to a unit standard deviation. Oscillations can be observed in the signals corresponding to controllers PC1653, PC651, PC652, PC653, LC652, PC670, PC1652, PC671, PC672, PC673, LC653 and LC654.

Figure 4.4. The measurements of the PVs in the drying section (publication I)

4.4.1 Variable subset selection

The aim of this procedure is to select the most pertinent variables to the fault. Consequently, it enables to reduce the dimensionality of the analysis, improve the results and facilitate their interpretation (Bauer et al., 2005b; Yuan & Qin, 2013). Several clustering methods are available for isolating faulty variables for diagnostic purposes, e.g., principle component analysis (Yuan & Qin, 2013; Zhao & Wang, 2016), spectral and oscillation analysis (Bauer et al., 2005b), spectral envelope method (Duan et al., 2014a), variable selection method using least absolute shrinkage and selection operator (Yan & Yao, 2015), reconstruction-based contribution method (Alcala & Qin, 2009; Li et al., 2016), sparse exponential discriminant analysis (Yu & Zhao, 2018) and more. In this case, due to the oscillatory behavior of the signals, the power spectra of the series (Fig. 4.5) was inspected in order to detect measurements with similar spectral behavior. The results show that the most prominent oscillation occurs at approximately 0.07 on the frequency axis (i.e., at ≈ 0.007 Hz) corresponding to $1/0.07 \approx 14$ samples per cycle. The controllers that oscillate at this frequency are : PC1653, PC651, PC652, PC653, LC652, PC670, PC1652, PC671, PC673, and LC653. Therefore, only those controllers are considered in the causal analysis.

Figure 4.5. The spectra of the time series (F_s is the sampling frequency = 0.1Hz) (The spectra of PC1652 is shown in red) (publication I)

In summary, this chapter focused on the thesis process case study. The board machine, its control strategy and its drying section were presented and described in detail. The process cases study involves valve stiction in one of the pressure controllers of the drying section and manifests as an oscillatory behavior of the controllers. The times series corresponding the controlled variables of the drying section were inspected and the spectra of the series was used in order to select the subset of variables for the causality analysis. Based on the spectral analysis, the frequency at which the controllers were oscillating was revealed and the controllers that share the same oscillation frequency were identified.

5. Results of the hybrid causal analysis

In this chapter the results of the hybrid causal analysis using each of the causality estimators are reported and analyzed. The causal analysis aims to identify the propagation path of the oscillation that originated in controller PC1652 due to valve stiction. Each estimator was implemented according to its developed methodology presented in Chapter 3. In addition, the parameters settings and the statistical evaluations of the results are discussed. Finally, the causality estimators are compared and evaluated based on several aspects.

5.1 Granger causality and frequency domain measures

Jiang et al. (2008) define a direct interaction from controller i to controller j if the control output (OP) of controller i can directly affect the controlled variable (PV) of controller j . According to this concept, the GC analysis was applied by evaluating the effect of the OPs on the process PVs in the drying section. The MVAR model was estimated using the least squares method and model order was chosen based on the AIC criteria ($p = 10$). The stationarity of the series was evaluated by testing for 'unit roots' according to the Augmented Dicky-Fuller (ADF) test (Seth, 2010). The time series that were found to be non-stationary were differentiated once (i.e., $x'(t) = x(t) - x(t - 1)$) and their stationarity was later confirmed by the ADF test. The statistical significance was evaluated according to the F -statistic test (Granger, 1969) and the results were corrected using the Bonferroni correction with a p -value of 0.01 (Seth, 2010).

The initial GC causality matrix is shown in Fig. 5.1. Each (i, j) entry in the matrix represents the GC from $OP(i)$ to $PV(j)$ while zeros correspond to GC values that didn't pass the F -statistic test. The next step is the refinement of the causality matrix which is performed according to the procedure described in Section 3.3. The refined causality matrix is shown in Fig. 5.2 and the corresponding causal model is shown in Fig. 5.3. In the refined matrix, the GC values which correspond

to indirect physical paths based on the connectivity matrix were set to zero. The refinement procedure using the search algorithm was able to eliminate most of the redundant results from the GC analysis. Approximately 88% of the spurious results from the initial causality matrix were eliminated, herewith affirming the efficacy of the proposed methodology.

	PC1653	PC651	PC652	PC653	PC670	LC652	PC1652	PC671	LC653	PC673
PC1653	-	0	0.072	0	0	0	0	0	0.028	0
PC651	0.039	-	0.056	0	0	0	0	0	0	0
PC652	0.065	0.016	-	0	0	0	0	0	0	0
PC653	0.014	0.019	0.017	-	0.017	0	0.024	0.018	0	0
PC670	0.018	0.029	0.031	0	-	0	0.018	0	0	0
LC652	0	0	0	0	0	-	0	0	0	0
PC1652	0.024	0.013	0	0.016	0.018	0	-	0.113	0.044	0.032
PC671	0	0	0	0.016	0.029	0	0.144	-	0.074	0.031
LC653	0.105	0.013	0.014	0.015	0	0.068	0.019	0.021	-	0.012
PC673	0	0	0	0	0	0	0	0	0	-

Figure 5.1. The initial GC causality matrix (publication I)

	PC1653	PC651	PC652	PC653	PC670	LC652	PC1652	PC671	LC653	PC673
PC1653	-	0	0	0	0	0	0	0	0	0
PC651	0	-	0.056	0	0	0	0	0	0	0
PC652	0.065	0.016	0	0	0	0	0	0	0	0
PC653	0	0	0	-	0.017	0	0	0	0	0
PC670	0	0.029	0.031	0	-	0	0	0	0	0
LC652	0	0	0	0	0	-	0	0	0	0
PC1652	0	0	0	0	0	0	-	0.113	0.044	0
PC671	0	0	0	0.016	0.029	0	0.144	-	0.074	0
LC653	0	0.013	0.014	0	0	0.068	0	0	-	0
PC673	0	0	0	0	0	0	0	0	0	-

Figure 5.2. The refined causality matrix. Highlighted values denote causality which is suspected to be spurious (publication I)

Yet, several spurious results remained in the model (denoted by the dashed arcs in the causal model (Fig. 5.3) and the highlighted entries in the refined causality matrix (Fig. 5.2)). LC653 discharges condensate into CT3 whose steam outlet is discharged into SG1, hence, affecting the pressure controllers PC651 and PC652. However, LC653 primarily affects the level in C3 and its affect on PC651 and PC652 is assumed to be secondary. Similarly, PC1652 primarily affects the pressure in SG3 rather than the level in C4, thus, its interaction with PC671 is significantly higher than with LC653. Furthermore, the causal model suggests two possible root causes: PC652 and PC671 since they are the only controllers

Figure 5.3. The causal model based on the refined GC causality matrix. Dashed arcs denote causality which is suspected to be spurious (publication I)

that have causal pathways to the rest of the controllers. Consequently, in order to obtain further insights on the level of interactions among the controllers in the drying section and to isolate the root cause, frequency domain analysis was implemented as an auxiliary step. The PDC represents direct causal effects, hence, it was utilized to identify the most powerful interactions and eliminate weak / indirect arcs from the causal model. On the other hand, the DTF which measures the total effects of one variable on another, was used to isolate the root cause. The PDC and the DTF were calculated based on the MVAR models which were previously estimated in the GC analysis. The diagonal terms of the noise covariance matrix differed by an order of magnitude, thus, the PDC and DTF were calculated according to Eqs. 2.19 and 2.20, respectively. The statistical significance of the PDC and the DTF was evaluated using the CFTd and CFTf surrogates (Faes et al., 2010), respectively. The significance level for each computed value at each frequency was set as the 95th percentile of the empirical distribution of the PDC / DTF obtained from 100 sets of surrogates. The PDC grid of plots is shown in Fig. 5.4.

The results of the PDC confirm that the interactions $LC653 \rightarrow PC652$, $LC653 \rightarrow PC651$ and $PC1652 \rightarrow LC653$ which were assumed to be ambiguous are indeed insignificant or indirect since at most frequencies their PDC values do not exceed their threshold for significance. The DTF represents the total variation that is transferred between two variables through direct and indirect paths (Gigi & Tangirala, 2010). Consequently, by summing the DTF values originating from each variable to all the others, one can identify the variable which mostly 'contributed' to the variation in the process. Moreover, the spectral analysis (Fig. 4.5) reveals that the process oscillates primarily at the frequency

Figure 5.4. The PDC values (blue lines) at each frequency between each pair of variables in the causal model and their corresponding threshold for significance estimated by the CFTd surrogates (red lines). *x*-axis: frequency (Hz), *y*-axis: magnitude of the PDC (publication I)

of 0.007 Hz (0.07 on the *x*-axis), thus, the DTF values at this frequency should reflect the highest 'contribution' to the variation in the process originating from each variable.

Fig. 5.5 shows the sum of the magnitude of the DTF originating from each variable at the frequency of 0.007 Hz. The DTF results clearly identify PC1652 as the root cause of the oscillation. Furthermore, as expected, the controllers in DG3 (PC1652, PC671 and LC653) are primarily responsible for to the energy transfer in the process.

Finally, based on the frequency analysis and the GC results, Fig. 5.6 illustrates the propagation path of the oscillation originating in PC1652. The oscillation initially propagated within DG3 to PC671 and then LC653. From DG3 the oscillation continued towards the consecutive drying groups (DG2 and DG1).

In summary, the GC analysis was successfully able to produce a fairly accurate causal model with a moderate effort. However, despite the refinement procedure incorporating the process connectivity information, few ambiguous results remained in the model. The frequency analysis was essential to locate the root cause and obtain further insights on the interactions among the controllers in the drying section.

Figure 5.5. Sum of the magnitude of the DTF originating from each variable at the frequency of 0.007 Hz (publication I)

5.2 Transfer entropy

5.2.1 Parameters settings

Selecting the TE parameters is a crucial step in the implementation since it affects both the results accuracy and the computational burden. Bauer et al. (2007a) provided guidelines for selecting the optimal parameters based on a reference case study. Accordingly, the initial prediction horizon (h) and time interval (τ) were set based on the suggestion of Bauer et al. (2007a). Then, the embedding dimensions were selected based on the guidelines provided by Duan et al. (2013). For each variable, j , the embedding dimension was determined by calculating the differential conditional TE for different embedding dimensions. Finally, for each pair of variables (i, j) , the differential $TE_{i \rightarrow j}$ was calculated for different embedding dimensions of i . The selected embedding dimensions are the minimum in which the change rate of the differential conditional entropy and TE do not vary significantly (Duan et al., 2013).

The selected parameters can be also used for the DTE / NDTE calculations. Therefore, the inclusion of intermediate variables in the DTE calculations does not increase the computational effort with respect to parameters estimation (Duan et al., 2013).

Figure 5.6. The causal model based on GC and frequency domain analysis (publication I)

5.2.2 Results

The TE implementation follows the methodology described in Section 3.3. The analysis was applied to the PVs according to the recommendations provided by Duan et al. (2013) and the PDFs were estimated by kernel estimation method (Eq. 2.30). Similarly to the GC analysis, the stationarity was tested with the ADF test (Seth, 2010). Two series whose set-points were modified during the investigated period were found to be non-stationary and were differentiated. Table 1 presents the calculated TE values between each pair of PVs when applied without the search algorithm. The calculated values did not undergo a statistical evaluation, hence, the results interpretation is difficult since most values are relatively high (>0.8) making it impossible to exclude indirect or spurious causality. Thus, obtaining a decent causal model with the TE method alone without calculating a statistical threshold is nearly impossible.

Table 5.1. The calculated TE among all PVs. (publication II)

$TE_{row \rightarrow column}$	PC1653	PC651	PC652	PC653	PC670	LC652	PC1652	PC671	LC653	PC673
PC1653	-	0.914	0.937	0.938	1.038	0.787	0.390	0.878	0.817	1.009
PC651	1.142	-	0.961	0.887	0.855	0.778	0.418	0.799	0.824	0.951
PC652	1.138	0.837	-	0.762	0.929	0.793	0.428	0.744	0.811	0.969
PC653	0.892	0.819	0.770	-	0.865	0.702	0.467	0.793	0.756	0.862
PC670	1.049	0.830	0.761	0.879	-	0.783	0.503	0.994	0.835	0.959
LC652	0.917	0.865	0.870	0.921	0.827	-	0.409	0.921	0.819	0.903
PC1652	0.983	0.900	0.836	0.831	0.871	0.773	-	1.100	0.754	0.785
PC671	0.967	0.903	0.822	1.132	0.895	0.760	0.513	-	0.996	0.911
LC653	1.095	0.877	0.823	0.932	1.197	0.859	0.554	0.654	-	0.945
PC673	0.926	0.843	0.820	0.768	0.840	0.739	0.374	0.788	0.762	-

Tables 5.2 and 5.3 show the TE and NTE values, respectively, when applied in conjunction with the search algorithm according to phase I in the procedure presented in Fig. 3.6. Namely, the TE / NTE were calculated only if two

controllers are connected by a direct path according to the search algorithm. Zero elements indicate on absence of physical connectivity between the controllers or that the controllers are connected indirectly. As expected, there is a strong correlation between the NTE and TE values: high TE values correspond to high NTE values and vice versa.

Table 5.2. The calculated TE values between each of the controllers according to phase I of the scheme presented in Fig. 3.6. The bold values denote causality that is suspected to be spurious or indirect. (publication II)

$TE_{row \rightarrow column}$	PC1653	PC651	PC652	PC653	PC670	LC652	PC1652	PC671	LC653	PC673
PC1653	-	0	0	0	0	0	0	0	0	0
PC651	0	-	0.961	0	0	0	0	0	0	0
PC652	1.138	0.837	-	0	0	0	0	0	0	0
PC653	0	0	0	-	0.865	0	0	0	0	0
PC670	0	0.830	0.761	0.879	-	0.783	0	0	0	0
LC652	0.917	0.865	0.870	0	0	-	0	0	0	0
PC1652	0	0	0	0	0	0	-	1.100	0.754	0
PC671	0	0	0	1.132	0.895	0	0.513	-	0.996	0
LC653	0	0.877	0.823	0	0	0.859	0	0	-	0
PC673	0	0	0	0.768	0.840	0	0	0	0	-

Table 5.3. The calculated NTE values between each of the controllers according to phase I of the scheme presented in Fig. 3.6. The bold values denote causality that is suspected to be spurious or indirect. (publication II)

$NTE_{row \rightarrow column}$	PC1653	PC651	PC652	PC653	PC670	LC652	PC1652	PC671	LC653	PC673
PC1653	-	0	0	0	0	0	0	0	0	0
PC651	0	-	0.089	0	0	0	0	0	0	0
PC652	0.102	0.108	-	0	0	0	0	0	0	0
PC653	0	0	0	-	0.180	0	0	0	0	0
PC670	0	0.107	0.068	0.108	-	0.079	0	0	0	0
LC652	0.077	0.100	0.076	0	0	-	0	0	0	0
PC1652	0	0	0	0	0	0	-	0.107	0.062	0
PC671	0	0	0	0.135	0.174	0	0.021	-	0.078	0
LC653	0	0.116	0.078	0	0	0.098	0	0	-	0
PC673	0	0	0	0.091	0.163	0	0	0	0	-

Fig. 5.7 presents the causal model based on the TE / NTE results of phase I. The results did not undergo a statistical evaluation, hence, the arcs are colored according to their corresponding TE values: bold arcs correspond to $TE > 0.9$, dashed arcs correspond to $TE < 0.8$ and the remaining arcs correspond to $0.8 < TE < 0.9$. In addition, red arcs denote causality which is suspected to be either indirect or spurious. One reason for the mis-detection of direct causality (e.g., $PC673 \rightarrow PC653$, $PC673 \rightarrow PC670$) is the control mechanism of the pressure difference controllers that manipulate the steam discharge from the condensate tanks. The steam can be discharged via two control valves in the steam outlet of each condensate tank. However, typically, only one valve is opened and the second valve is opened only if a high pressure difference is needed between the condensate tanks and the steam cylinders. This scenario demonstrates that physical connectivity does not always indicate causality.

Consequently, in phase II, the DTE / NDTE are calculated for those interactions which are suspected to be spurious or indirect (denoted by the red arcs in Fig. 5.7).

Figure 5.7. The initial causal model based on the TE/NTE results obtained in phase I. Bold arcs correspond to TE values higher than 0.9 while dashed arcs correspond to TE values lower than 0.8. The red arcs indicate that causality can be detected but is suspected to be either indirect or spurious. (publication II)

The search algorithm is utilized in phase II in order to retrieve all the available physical pathways between each pair of controllers. Then, the DTE and the NDTE are calculated for each indirect path. For example, consider the connectivity from LC652 to PC1653. According to the output of the search algorithm (Fig. 5.8) five propagation path are found from LC652 to PC1653. Two of the paths are indirect: $LC652 \rightarrow PC652 \rightarrow PC1653$ (path 5) and $LC652 \rightarrow PC651 \rightarrow PC652 \rightarrow PC1653$ (paths 3 & 4) while paths 1 and 2 are direct. Thus, the DTE is calculated twice: once with PC652 as an intermediate variable and once with PC651 and PC652 as intermediate variables. Note that the search algorithm only retrieves the paths which traverse controllers that are part of the investigation.

Checking cause and effect relationship between LI-652 and PI-1653...

LI-652 is connected to C-3. There are 5 feasible propagation paths from C-3 to PI-1653...

Path 1 is	Path 2 is	Path 3 is	Path 4 is	Path 5 is
C-3	C-3	C-3	C-3	C-3
LI-652	LV-652	SG1_Steam_Line	SG1_Steam_Line	SG1_Steam_Line
LC-652	C-2	PI-651	PI-651	SG-1
LV-652	PI-1653	PC-651	PC-652	PI-652
C-2		PV-651	PV-652	PC-652
PI-1653		SG-1	C-2	PV-652
		PI-652	PI-1653	PI-1653
		PC-652		
		PV-652		
		C-2		
		PI-1653		

Figure 5.8. Finding physical pathways between $LC652 \rightarrow PC1653$ using the search algorithm. LI=Level Indicator, LV=Level Transmitter, PI=Pressure Indicator, PV- Pressure Transmitter , PC=Pressure Controller, LC= Level Controller (publication II)

Table 5.4. The calculated DTE/NDTE values for the indirect paths in the initial model. (publication II)

	DTE	NDTE	Indirect pathways
$PC673 \rightarrow PC653$	0.571	0.764	$PC673 \rightarrow PC670 \rightarrow PC653$
$PC673 \rightarrow PC670$	0.706	0.707	$PC673 \rightarrow PC653 \rightarrow PC670$
$PC1652 \rightarrow LC653$	0.137	0.291	$PC1652 \rightarrow PC671 \rightarrow LC653$
$LC653 \rightarrow PC651$	0.236	0.595	$LC653 \rightarrow LC652 \rightarrow PC651$
	0.070	0.207	$LC653 \rightarrow LC652 \rightarrow PC652 \rightarrow PC651$
$LC653 \rightarrow PC652$	0.187	0.408	$LC653 \rightarrow PC651 \rightarrow PC652$
	0.212	0.553	$LC653 \rightarrow LC652 \rightarrow PC652$
$LC652 \rightarrow PC651$	0.266	0.726	$LC652 \rightarrow PC652 \rightarrow PC651$
$LC652 \rightarrow PC1653$	0.291	0.423	$LC652 \rightarrow PC652 \rightarrow PC1653$
	0.070	0.112	$LC652 \rightarrow PC651 \rightarrow PC652 \rightarrow PC1653$

The calculated values of the DTE and NDTE for all the indirect paths based on the results of phase I are displayed in Table 5.4. Based on the results, the causality from PC673 to PC653 and PC670 should be considered as direct due to the high values of DTE and NDTE. PC670 controls the steam outlet from C8 which is partially discharged into SG2, thus, affecting the pressure controllers in DG2. However, it is unlikely that those pathways reflect the propagation of the oscillation originated in PC1652. Moreover, based on the initial model (Fig. 5.7) PC1652 has causal pathways to all the controllers except PC673. Therefore, although there might be a causal effect from PC673 to PC653 and PC670 it most likely does not reflect the fault propagation path since no oscillation was observed in the other pressure controller of SG7, PC659. This assumption is also supported by the GC results (Fig. 5.2) where no causality that originated in PC673 could be identified.

The DTE and NDTE values for $PC1652 \rightarrow LC653$ are relatively low, therefore, the causality can be considered as weak or indirect. In addition, the results imply a certain level of causality from LC653 to PC651 and PC652 (although the DTE values are quite low compared with the NDTE values). However, LC653 primarily affects the level of C3, thus, it is assumed that the affect of LC653 on the pressure controllers of DG1 is secondary (similarly to the results obtained in the GC analysis).

The causality from LC652 to PC651 and PC1653 can be considered as direct since both DTE and DNTE values of the paths $LC652 \rightarrow PC652 \rightarrow PC651$ and $LC652 \rightarrow PC652 \rightarrow PC1653$ are relatively high. The steam outlet of C3 is directly discharged to the steam line of SG1, hence, it affects all the pressure controllers of DG2: PC651, PC652 and PC1653. The final model illustrating the propagation path of the oscillation originated in PC1652 is shown in Fig. 5.9. The model reveals the strong coupling between the pressure controllers in the drying section. The TE method is invariant to the time delay, thus, it is difficult to estimate how fast the oscillation propagated within the controllers. However, it is

reasonable to assume that the oscillation propagated faster among the pressure controllers due to the strong mutual interactions between the pressure and the pressure difference controllers in each DG. Moreover, the causal model reveals that the oscillation propagated to all the pressure controllers in the successive DGs, however, only two level controllers were affected by the fault. Thus, the oscillation had a stronger effect on the pressure controllers rather than the level controllers in the drying section.

Figure 5.9. The final causal model based on TE analysis illustrating the propagation path of valve stiction in PC1652 (publication II)

To conclude, the two-phase methodology based on TE was successfully applied to the current case study and was able to capture the causal dependencies among the control loops in the drying section. The findings of this study suggest that the DTE has a vital role in excluding indirect pathways from the initial model obtained in phase I. Therefore, it seems that the application of the bivariate TE is limited to small-scale systems with a simple topology. Furthermore, when investigating highly inter-connected systems, it is essential to use the information on the process connectivity for facilitating the TE analysis and obtaining reliable results. Alternatively, a large system can be divided into smaller sub-systems in order to reduce the dimensionality of the analysis.

The most important limitation of this study lies in the fact that the results of the TE / DTE were not tested for statistical significance. Due to the difficulty and complexity of constructing the surrogate data (Duan et al., 2013), the results were evaluated according to their magnitude. However, since the information on the process connectivity was incorporated into the analysis, the final causal model is fairly accurate. Yet, further studies need to be carried out in order to establish a statistical threshold with a high confidence level. In addition, the selection of the indirect paths from the initial model obtained in phase I to be evaluated for direct causality in phase II required careful attention and basic process knowledge.

Thus, it remains a challenge to develop a fully automated causal analysis without utilizing human process knowledge to validate the results.

5.3 Nearest neighbors

5.3.1 Parameters settings

The parameters for the NN implementation were estimated based on the guidelines provided by Bauer et al. (2007b). The embedding dimension was selected by plotting $H_{x \rightarrow y}$ for each pair of variables while m was varied from 1 to 10 and $k = h = 1$. The value of m for which $H_{x \rightarrow y}$ reached its maximum value was selected for each pair of variables. Next, the same procedure was repeated while varying k from 1 to 10, $h = 1$ and m was set to its optimal value according to the previous step. Finally, the procedure was repeated when h varied from 1 to 10 and k and m were kept at their optimal settings according to the previous steps. An example for selecting the parameters of the pair $PC651 \rightarrow PC652$ is shown in Fig. 5.10.

Figure 5.10. NN parameters setting for $PC651 \rightarrow PC652$ ($N = 3000, K = 200$). $H_{PC651 \rightarrow PC652}$ is plotted when m , k and h are varied (upper, middle and lower panels, respectively). The chosen parameters are circled. (publication III)

The upper panel presents the value of $H_{PC651 \rightarrow PC652}$ when m is varied and $h = k = 1$, the middle panel shows the value when k is varied and m and h are

fixed and the bottom panel shows the value when h is varied and m and k are fixed according to their selection in the upper panels. The selected parameters are obtained when $H_{PC651 \rightarrow PC652}$ reaches a maximum.

The number of nearest neighbors, K , is typically chosen to be equal to the number of cycles present in the analyzed data in case of an oscillatory disturbance (Bauer et al., 2007b). In this case, 3000 samples were analyzed and since the oscillation period is 14 samples (Fig. 4.5), K was set to 200.

5.3.2 Results

The directionality measures obtained in phase I are presented in Table 5.5. Empty cells indicate on either lack of direct physical connectivity between the row and column controllers or that the directionality is in the opposite direction (only positive values are presented).

Table 5.5. Results of phase I: Initial causality matrix based on NN method (publication III)

$H_{row \rightarrow column}$	PC1653	PC651	PC652	PC653	PC670	LC652	PC1652	PC671	LC653	PC673
PC1653	-	-	-	-	-	-	-	-	-	-
PC651	-	-	0.082	-	-	-	-	-	-	-
PC652	-	0.178	-	-	-	-	-	-	-	-
PC653	-	-	-	-	0.978	-	-	-	-	-
PC670	-	1.802	1.384	0.572	-	1.261	-	-	-	-
LC652	-	0.217	0.101	-	-	-	-	-	-	-
PC1652	-	-	-	-	-	-	-	1.206	2.593	-
PC671	-	-	-	-	0.326	-	-	-	0.738	-
LC653	-	1.792	0.587	-	-	1.556	-	-	-	-
PC673	-	-	-	0.448	-	-	-	-	-	-

In phase II of the analysis, each value in the initial causality matrix is further investigated by calculating the MV directionality according to the newly proposed measure (Eqs. 3.1-3.2). First, a new connectivity matrix is constructed from the initial causality matrix according to the logic described in Fig. 3.8. Then, the MV directionality measure is calculated for each indirect path based on the new connectivity matrix. The outcome is a causality matrix where '1' signifies a direct causality between the row and column elements while the rest of the values correspond to the mean of the MV directionality measure of all the indirect paths between the row and column elements based on the new connectivity matrix. The final causality matrix is presented in Table 5.6.

For exemplifying the methodology, consider the directionality $PC670 \rightarrow PC651$. The initial causality matrix (Table 5.5) indicates that $H_{PC670 \rightarrow PC651} = 1.802$. According to the new connectivity matrix, the search algorithm finds three indirect paths from PC670 to PC651. For each path, the MV directionality measure is calculated according to Eqs. 3.1 - 3.2 (the results are summarized in Table 5.7). The mean value of all the measures is 0.282 (see Table 5.6) which is significantly

Table 5.6. Results of phase II of the NN analysis (publication III)

$H_{row \rightarrow column}$	PC1653	PC651	PC652	PC653	PC670	LC652	PC1652	PC671	LC653	PC673
PC1653	-	-	-	-	-	-	-	-	-	-
PC651	-	-	1	-	-	-	-	-	-	-
PC652	-	1	-	-	-	-	-	-	-	-
PC653	-	-	-	-	1	-	-	-	-	-
PC670	-	0.282	0.270	1	-	1	-	-	-	-
LC652	-	0.084	0.017	-	-	-	-	-	-	-
PC1652	-	-	-	-	-	-	-	1	0.673	-
PC671	-	-	-	-	1	-	-	-	1	-
LC653	-	0.148	0.078	-	-	1	-	-	-	-
PC673	-	-	-	1	-	-	-	-	-	-

higher than zero (in this study, values > 0.1 are considered as significant), thus, it can be deduced that the causality from PC670 to PC651 is indeed direct.

Table 5.7. The indirect paths from PC670 to PC651 and their MV directionality measure based on NN method (publication III)

Indirect Path	The MV directionality measure
$PC670 \rightarrow PC652 \rightarrow PC651$	0.339
$PC670 \rightarrow LC652 \rightarrow PC651$	0.338
$PC670 \rightarrow LC652 \rightarrow PC652 \rightarrow PC651$	0.169

The rest of the results of phase II show that $H_{PC670 \rightarrow PC652}$, $H_{PC1652 \rightarrow LC653}$, $H_{LC653 \rightarrow PC651}$ are all > 0.1 , hence, they indicate on direct causality. However, the values of $H_{LC652 \rightarrow PC651}$, $H_{LC652 \rightarrow PC652}$ and $H_{LC653 \rightarrow PC652}$ are < 0.1 , thus, they indicate either indirect or insignificant level of causality (the corresponding values appear bold in Table 5.6). Accordingly, the final causal model depicting the propagation path of the oscillation originated in PC1652 is illustrated in Fig. 5.11.

Figure 5.11. The final causal model based on NN method (dashed arcs correspond to causality which is indirect or spurious while the dotted arcs corresponds to causality which is direct but had not been identified) (publication III)

The dashed arcs denote interactions that are considered as spurious or indirect based on process knowledge and the previous results obtained from the GC and TE investigations. For instance, the directionality from PC673 to PC653 has

been identified as direct, however, as mentioned earlier, this ambiguous causality is due to the control mechanism of the pressure difference controllers in the drying section. PC673 manipulates two control valves at the steam outlet of C8 whereas only one valve is constantly open and the second one is opened only if a higher pressure is needed. Thus, although the search algorithm finds a direct physical path from PC673 to PC653, if the connecting valve is closed, there is no information transfer between the controllers. In addition, the directionality from PC652 to PC1653 and from PC671 to PC1652 had not been identified (unlike the GC and TE results). However, overall the analysis demonstrates a high level of accuracy ($\sim 90\%$).

To sum up, the proposed methodology based on the NN method offers a practical and efficient way to do causal analysis due to its ability to discriminate between direct and indirect interactions. Consequently, the results are easy to interpret and the computational effort is reduced since the directionality measure is calculated based on the type of connectivity. Furthermore, the newly proposed MV measure for estimating direct causality proved to be beneficial in excluding indirect interactions in phase II of the analysis. Although the results of phase I might be sufficient to obtain a satisfactory causal model and to locate the root cause, phase II is an essential step since physical connectivity does not necessarily imply direct causality. Ultimately, the two-phase analysis yields a highly credible causal model although the results were not tested for statistical significance. This enables to retrace the propagation path with less computational effort compared with other methods which require surrogate data in order to validate the results. On the other hand, since the results did not undergo a statistical evaluation several ambiguous arcs remained in the final model. Thus, in future cases it is advised to utilize process knowledge, if available, to validate the results.

5.4 NPMR-based causality estimator

5.4.1 Parameters settings

The time delay, τ , was estimated as the time when the autocorrelation function reaches $1/e$ as suggested by Nicolaou & Constandinou (2016). The estimated delay for the majority of the series was 3s, and therefore τ was set to 3 for the entire analysis. The embedding dimension was evaluated according to the method proposed by Cao (1997): while d was varied from 1 to 10 and $\tau = 3$, the d for

which the values of $E1$ and $E2$ stopped changing was selected as the embedding dimension. Based on the results, d was set to 4 throughout the analysis.

Lastly, the kernel tolerance was tuned for each pair of variables by calculating the model fit (Eq. 2.44) for $\sigma = 0.2, 0.4, 0.6, \dots, 2$ with $\tau = 3$ and $d = 4$. The tolerance for which the best model fit was obtained was selected for each pair. The optimal value of σ for each pair varied between 0.2-0.8, therefore each pair was assigned with a unique value of σ throughout the analysis. Figure 5.12 presents the model fit as a function of σ when PC1652 is used as predictor for the rest of the controllers. The results indicate that the best model fit is obtained at low values of sigma (0.2-0.8). Moreover, as expected, the best fitting model is obtained when predicting the neighboring controllers: PC671, PC653, PC670 and LC653 .

Figure 5.12. The model fit for different values of σ with $\tau = 3, d = 4$ when PC1652 is used as predictor for all other controllers (publication IV)

5.4.2 Results

The analysis was carried out according to the logic described in Figure 3.10. The statistical significance of the estimations was evaluated using AAFT surrogates. 20 surrogates were generated for each causality estimation. Then, for each pair of surrogates, the NPMR-based causality was applied and the significance level was set to the maximum value of C_{NPMR} of all estimations.

The causality matrix with the C_{NPMR} values between each pair of controllers is shown in Table 5.8 (only positive values are shown in the causality matrix). In addition, empty cells indicate a lack of physical connectivity or C_{NPMR} values that did not exceed their threshold for significance level.

Table 5.9 presents the type of connectivity between each pair of controllers as identified by the search algorithm: empty cells indicate on lack of physical connectivity between the row and column elements, squares denote indirect connectivity and bullets denote direct connectivity. According to Tables 5.8 - 5.9,

all the paths which were considered as indirect by the search algorithm (i.e., denoted by the squares in Table 5.9) appear as empty cells in the causality matrix. Thus, their corresponding C_{NPMR} values show indirect or lack of causality as well. The majority of paths which were identified as direct by the search algorithm (i.e., denoted by the bullets in 5.9) were established as direct as well by their corresponding C_{NPMR} values. In this study, a discrepancy between the physical connectivity and the causality estimation can occur due to one of the following reasons: causality might exist but on a low level (e.g., $LC652 \rightarrow PC1653$) or there is a direct physical path but no information transfer due to a closed valve. The latter scenario is the case with $PC673 \rightarrow PC653$ and $PC673 \rightarrow PC670$. In this case, the C_{NPMR} results properly indicate that the causality originating in PC673 is spurious. Once more, this exemplifies that physical connectivity does not necessarily imply causality.

The causal model according to Table 5.8 is shown in Fig. 5.13. Several arcs were suspected as indirect and are therefore denoted as dashed arcs.

The path $PC1652 \rightarrow LC653$ is initially suspected as indirect based on the captured topology. Furthermore, according to the GC and TE results, the causality from PC1652 to LC653 was assumed to be indirect. However, according to the search algorithm the physical path from PC1652 to LC653 is direct since the condensate from SG3 is directly transferred to C4. Moreover, the high C_{NPMR} value (0.498) suggests that the causality from PC1652 to LC653 is indeed direct.

The causality from LC653 to PC651 and PC652 is suspected as indirect as well based on the captured topology. The search algorithm indicates that the direct connectivity from LC653 to PC651 and PC652 is due to the steam outlet of C3 (see the output of the algorithm for $LC653 \rightarrow PC651$ in Figure 5.14).

However, since the liquid outlet of C4 primarily alters the level of C3, similarly to the previous investigations, it is suspected that the causality from LC653 to PC651 and PC652 is indirect via LC652. Consequently, the C_{NPMR} of $LC653 \rightarrow PC652$ and $LC653 \rightarrow PC651$ via the intermediate controller LC652 are calculated (see the results in Table 5.10). The results suggest that the causality from LC653 to

Table 5.8. The NPMR-based causality matrix with adjusted parameters (publication IV)

$C_{NPMR_{row \rightarrow column}}$	PC1653	PC651	PC652	PC653	PC670	LC652	PC1652	PC671	LC653	PC673
PC1653										
PC651			0.053							
PC652	0.065	0.172								
PC653					0.303					
PC670		0.036	0.078	0.156		0.100				
LC652		0.102	0.058							
PC1652								0.190	0.498	
PC671				0.094	0.134		0.090		0.234	
LC653		0.108	0.249			0.135				
PC673										

Table 5.9. The connectivity information: indication of direct / indirect paths according to the search algorithm (publication IV)

	PC1653	PC651	PC652	PC653	PC670	LC652	PC1652	PC671	LC653	PC673
PC1653										
PC651	□		•							
PC652	•	•								
PC653	□	□	□		•	□				
PC670	•	•	•	•		•				
LC652	•	•	•							
PC1652	□	□	□	□	□	□		•	•	
PC671	□	□	□	•	•	□	•		•	
LC653	□	•	•	□	□	•				
PC673	□	□	□	•	•	□				

* Empty cells denote lack of physical connectivity, squares denote indirect paths and bullets denote direct paths between the row and column elements

Figure 5.13. The causal model based on the NPMR-based causality estimation (dashed arcs correspond to causality which is suspected as indirect) (publication IV)

PC652 is indeed direct while the causality from LC653 to PC651 can be considered as indirect. Accordingly, the final causal model is illustrated in Figure 5.15.

Once more, the model identifies two possible root causes for the fault: PC1652 and PC671. Analogously to the approach presented in the frequency domain analysis (Fig. 5.5), the sum of the C_{NPMR} values originating from each controller was calculated. The aim of this procedure is to provide a quantitative estimation of the total influence of each variable on the remaining ones. The results (Figure 5.16) clearly identify PC1652 as the root cause. Moreover, as expected, the highest C_{NPMR} values originate from the controllers in DG3 (PC1652, PC671 and LC653) and decrease along the consecutive DGs in the drying section.

Overall, the analysis proved to be highly efficient and precise in identifying

Table 5.10. The indirect paths from LC653 to PC651 and LC652 and their NPMR-based causality estimation(publication IV)

Indirect Path	C_{NPMR}	Significance level
$LC653 \rightarrow LC652 \rightarrow PC651$	0.051	0.093
$LC653 \rightarrow LC652 \rightarrow PC652$	0.138	0.011


```

*****
Checking cause and effect relationship between LI-653 and PI-651...
LI-653 is connected to
C-4

There is a direct link between C-4 and PI-651...
The direct path is :

Path 1 is
C-4
LI-653
LC-653
LV-653
C-3
SG1_Steam_Line
PI-651

Path 2 is
C-4
LV-653
C-3
SG1_Steam_Line
PI-651

```

Figure 5.14. The output of the search algorithm for direct paths from LC653 to PC651. LI= Level Indicator, LC= level Controller, LV= Level Transmitter, PI= Pressure Indicator (publication IV)

Figure 5.15. The final NPMR-based causal model (publication IV)

the propagation path of the oscillation. Mis-detection might be attributed to parameters selection, in particular the kernel tolerance. When tuning the σ parameter, it was observed that a small variation in σ lead to a significant change in the corresponding C_{NPMR} value. In addition, it was observed that σ has a larger impact on C_{NPMR} than d and τ . Therefore, it remains a challenge for future investigations to optimize the selection procedure for σ .

On the other hand, modifying the parameters did not alter the pattern of the causality much but rather changed the amplitude of the C_{NPMR} values which lead to more false positive results. Table 5.11 presents C_{NPMR} values which were obtained via the same methodology presented in Fig. 3.10 but with fixed parameters ($\tau = 1, d = 4, \sigma = 1$). The values colored in red correspond to estimations which were excluded when using adjusted parameters (Table 5.8). The corresponding causal model is presented in Figure 5.17 where red arcs correspond to the red colored values in Table 5.11. The results using the fixed

Figure 5.16. The sum of all C_{NPMR} values originating from each controller (publication IV)

Table 5.11. The NPMR-based causality matrix with fixed parameters $\tau = 1, d = 4, \sigma = 1$ (publication IV)

$C_{NPMR_{row \rightarrow column}}$	PC1653	PC651	PC652	PC653	PC670	LC652	PC1652	PC671	LC653	PC673
PC1653										
PC651	0.206		0.269							
PC652	0.213	0.107								
PC653					0.633					
PC670	0.289	0.186	0.192	0.472		0.295				
LC652	0.228	0.082	0.236							
PC1652								0.407	0.588	
PC671				0.498	0.533				0.603	
LC653		0.238	0.275			0.317				
PC673					0.263					

parameters demonstrate that the causality pattern remains almost unaltered in comparison with the model obtained using the adjusted parameters, however, more false-positive results were obtained (denoted by the red arcs). In addition, the causality $PC671 \rightarrow PC1652$ which was accurately identified in the analysis with the adjusted parameters was not detected when using fixed parameters.

In conclusion, this study successfully extends the application of NPMR-based estimator to an industrial process. Although an appropriate selection of the parameters is highly recommended, it is not imperative in order to obtain satisfactory results. Setting initial parameters based on process knowledge (e.g., the time delay) can be sufficient to obtain an adequate model and locate the root cause.

Figure 5.17. The causal model obtained with fixed parameters (red arcs correspond to causality which was not obtained with adjusted parameters) (publication IV)

5.5 Comparison and evaluation of the causality estimators

Several investigations have been carried out into the current case study using different causality estimators according to the methodologies presented in Chapter 3. All the estimators have been applied in conjunction with the search algorithm which incorporates the information on the process connectivity into the analysis, thereby minimizes the number of spurious results in the causal model. The incorporation of the process connectivity in this case study was crucial for obtaining useful results due to the high connectivity between the controllers in the drying section. The estimators are evaluated and compared according to the following criteria: accuracy of the results and their interpretability, computational burden, statistical evaluation and industrial applicability. Table 5.12 presents a comparison between the different attributes of the causal methodologies presented in this thesis. While all the methods were applied as bivariate and / or multivariate analysis, only two of them are linear: the GC and frequency domain methods.

The GC is a straightforward method with a relatively low computational effort which is applied as a single step MV analysis. The GC method combined with the connectivity information produced fairly accurate results and was able to

Table 5.12. Comparison between the causality methodologies

Method	Bivariate	Multivariate	Linear	Non-linear	Parametric	Nonparametric	implementation phases	Remarks
Granger causality	✓	✓	✓	-	✓	-	1	Non-linear extensions exist but are not part of this study
Frequency domain analysis (PDC/DTF)	✓	✓	✓	-	✓	-	1	
Transfer Entropy	✓	✓	✓	✓	-	✓	2	MV implementation via the DTE (Duan et al., 2013)
Nearest neighbors	✓	✓	✓	✓	-	✓	2	MV implementation according to publication III
NPMR-based causality estimator	✓	✓	✓	✓	-	✓	1	

identify the fault propagation path. Yet, the frequency domain analysis was essential in order to further exclude ambiguous results and to locate the root cause. Ultimately, the frequency domain analysis along with GC resulted in a model with approximately 90% accuracy. Although the GC performance depends on the model estimation and the linearity of the investigated system, in this case, non-linear nonparametric methods such as NN and TE did not show superior results compared with the linear methods. This implies approximately linear relationships between the controllers in the drying section. Furthermore, the frequency domain analysis was proven to be highly effective and productive due to its ability to quantify the direct and indirect energy transfer between the variables at each frequency. Moreover, the application of the frequency domain methods is especially useful when the frequency of oscillation is known. The main limitation of the DTF / PDC is determining the statistical significance level using surrogate data which is strenuous since it requires calculation of a threshold value at each frequency. Consequently, it is advised to utilize the frequency domain measures as a supplementary analysis in case it is desired to obtain deeper insights into the system behavior or in order to locate the root cause. In the latter case, the root cause can be successfully isolated (as shown in Fig. 5.5) even if the results did not undergo a statistical evaluation.

The TE, NN and the NPMR-based estimators are all nonparametric, nonlinear and require the estimation of several parameters : prediction horizon, embedding dimension and time delay. The procedure for estimating the parameters is roughly similar for all the methods, however, the TE requires the estimation of the joint PDFs whose complexity increases with the dimensionality of the analysis. Thus, from a computational point of view, the TE is the most difficult to implement. Unlike NPMR, TE and NN are implemented in two phases: bivariate analysis in phase I and multivariate analysis is implemented in phase II in order to determine indirect causality. In addition, the TE and NN results were evaluated according to their magnitude instead of using computationally expensive methods involving surrogate data (Duan et al., 2014a). Though the TE and NN methods yielded a fairly accurate causal model, the TE method produced slightly more spurious results compared with the NN method. Moreover, the selection of the indirect paths for the DTE calculation in phase II was based on inspection of the captured topology in phase I and process knowledge unlike the NN method in which phase II is implemented automatically once the new connectivity matrix is constructed. Thus, when considering the computational burden and accuracy of the results, the NN is more practical for industrial applications where non-linear and computationally efficient methods are often desired.

The NPMR-based estimator demonstrated several advantages compared with the other estimators: aside from its inherent benefits of being nonparametric and not restricted to linear processes it showed superior accuracy compared to the NN and TE methods. Moreover, the NPMR-based estimator can be applied in a single step as either a bivariate or multivariate analysis without any modifications which makes it highly practical and beneficial for industrial applications. Moreover, the results are easy to interpret since all the estimations undergo a statistical significance test. Consequently, the analysis produced a highly accurate model with very few ambiguous results. In fact, the final results indicate that the analysis yielded only one specious result ($LC653 \rightarrow PC651$) which was identified by calculating the MV estimation ($LC653 \rightarrow LC652 \rightarrow PC651$). However, there was not significant difference in the ability to identify the propagation path when applying the conditional GC followed by the frequency domain analysis and the NPMR-based estimator. These findings are somewhat expected since the relationships between the feedback control loops in the drying section are fairly linear. Thus, in such cases, linear methods should be preferred in order to simplify the analysis. In addition, the NPMR-based estimator was able to locate the root cause by calculating the sum of C_{NPMR} of each row in the causality matrix. Thereby, the estimator can be easily used to validate or locate the root cause of a fault without using additional measures. To sum up, Table 5.13 presents a comparison between the different causal methodologies based on their implementation in the current study.

Table 5.13. Comparison between the causality estimators based on the results of the hybrid causal analysis

Method	Results accuracy	Parameters to select	Significance testing	Computational load	Remarks
Granger causality and the frequency domain measures	High ($\approx 88\%$ accuracy)	Model order (AIC criteria)	Yes (F -statistic test for the GC and CFTd and CFTf surrogates for the PDC and DTF, respectively.)	Low (The significance testing of the PDC and DTF using surrogate data requires high computational effort)	Frequency analysis was used as an auxiliary method to exclude spurious results and identify the root cause.
Transfer Entropy	Good	Embedding dimension, prediction horizon and time delay	No	High	The parameters estimation and analysis are very time consuming and complex due to the estimation of the PDFs
Nearest neighbors	High ($\approx 90\%$ accuracy)	Embedding dimension, prediction horizon, time delay and number of nearest neighbors	No	Moderate	
NPMR-based causality estimator	Very High (The highest among all estimators)	Embedding dimension, time delay and kernel tolerance	Yes (with AAFT surrogates)	Moderate	Most efficient non-linear method

In general, it seems that in future cases straightforward linear methods such as the cross-correlation or GC should be applied at first to obtain initial results, especially when investigating small-scale systems. In cases where the disturbance exhibits an oscillatory behavior, frequency domain analysis is desirable and preferred over the cross-correlation method. In particular, the GC has been formulated in the frequency domain in order to address oscillatory aspects in specific frequency bands (Ladroue et al., 2009). Then, additional spectral measures such as DTF / PDC can be used to obtain further insights into the system or to validate the initial results. If the investigated system is highly nonlinear or if the linear methods provide unsatisfactory results, nonlinear causality estimators based on NPMR or NN should be applied. The computational complexity of the TE is considerably larger due to the kernel estimation of the joint PDFs, especially when the number of intermediate variables for the DTE calculation increases. Thus, the TE method should not be used when the system is large in order to avoid the calculations of high-dimensional joint PDFs. Alternatively, a large-scale complex system can be broken into smaller sub-systems and thereafter analyzed within each sub-system (Duan et al., 2013). A reasonable approach to tackle a complex system could be to apply at least two different data-based methods (e.g., a linear and nonlinear) and fuse the results into a single model. Regardless, it is advised to verify the final results using process knowledge or site personnel if available. In conclusion, based on the results obtained in this thesis, Table 5.14 provides guidelines for selecting the appropriate method based on the system type and nonlinearity. The methods are listed according to their recommended implementation order. For instance, in a case of a large-scale system that is highly nonlinear, it is recommended to initially try the NPMR-based estimator and then if a second method is needed, the nearest neighbors method should be applied next.

Table 5.14. Guidelines for selecting causality estimator

Method	Small scale system	Complex / Large-scale system	Highly nonlinear	Linear / low order of nonlinearity	Remarks
Granger causality	✓	✓	-	✓	Spectral GC is preferred in case of an oscillatory disturbance
Frequency domain analysis (PDC/DTF)	✓	-	-	✓	Use only in case of an oscillatory disturbance
NPMR-based causality estimator	✓	✓	✓	✓	
Nearest neighbors	✓	✓	✓	✓	
Transfer Entropy	✓	-	✓	✓	

6. Summary and conclusions

This thesis presented a hybrid analysis for capturing process causality using several causality estimators combined with the information on the process connectivity. A causal methodology has been developed for each estimator by considering its specific characteristics. All the estimators were applied to an industrial case study of valve stiction in a board machine. The keystone of the hybrid analysis is the automatic consolidation of the connectivity information with the causality estimators using a specialized search algorithm. The analysis is designed to estimate the causality based on the physical connectivity, thereby, the computational effort is minimized. Moreover, the results indicate that it is vital to integrate the connectivity information with a data-based analysis in order to obtain adequate results, especially when investigating a highly inter-connected system. Consequently, the proposed hybrid causal analysis can efficiently address complex systems while simultaneously increasing the accuracy of the results and reducing the computational load. Furthermore, the possibility of capturing the process connectivity via CAD software and to automatically incorporate it into a data-based analysis using a search algorithm provides a practical and efficient diagnostic tool which is beneficial for industrial applications. In the future, the proposed approach can be used to study how different types of faults propagate within a system, thereby assist in selecting the critical variables to monitor and expedite the isolation of a fault root cause before it severely deteriorates the product quality.

The hypothesis of this thesis was that a hybrid causal analysis which automatically integrates information on the process connectivity with data-based methods provides an enhanced causal model which can serve as a basis for the development of a powerful FDD system. By referring to the results of the causal analysis presented in Chapter 5 and to their practical implications as well as to the discussion above, the hypothesis was verified.

A major limitation of this study is that the directionality is evaluated based on the process topology. On the one hand, the possibility of capturing the plant topology using CAD software offers a practical tool for automated causal analysis (Yim et al., 2006). On the other hand, the connectivity matrix is merely a qualitative representation of the process schematic which does not include any information on the process itself, e.g., chemical composition of the components, reactions rates, etc. Therefore, it is problematic, for instance, to retrace the propagation path of disturbances which cause variations in the composition of a stream. One approach to tackle this problem could be to label the contents of vessels and pipes with the attribute of composition (Thambirajah et al., 2009). Addressing various limitations of process schematics is further discussed by Thambirajah et al. (2009) and Yim et al. (2006). Further studies should therefore concentrate on automatic techniques to deal with unmeasured variables. Moreover, the development of standardized software which could discover and examine additional information on the process such as mathematical models of reactions or feed composition changes that effect the process can enhance the connectivity information and thereby the ability to construct a causal model (Thambirajah et al., 2009).

Another issue that was not addressed in this study is the statistical significance of the TE/ DTE and the NN results. Generally, it is complex to construct surrogate data (Bauer et al., 2007a) or resampling data (Vakorin et al., 2009) which complies with the null hypothesis, especially in the case of DTE (Duan et al., 2013). Thus, the results were evaluated according to their magnitude in this thesis. Consequently, several indirect or spurious results remained in the final model. However, by virtue of the search algorithm, both the TE and NN final results showed a relatively high level of accuracy. This exemplifies that the process connectivity information can be utilized to validate the results of a data-based causal analysis instead of using computationally expensive methods. Yet, future work is needed to establish a statistical threshold with a high confidence level. In particular, an efficient and accurate PDF estimation needs to be developed as an alternative to the kernel estimation method.

A natural progression of this work is to analyze the efficacy of each of the causality estimators using other case studies with different types of disturbances. In particular, the following aspects should be taken into account:

- Non-linearity of the system (e.g., testing systems with a high order of non-linearity)

- Complex / large-scale systems with multiple bidirectional and recycle streams.
- Different types of faults and disturbances: e.g., sensor faults, non-oscillatory disturbances, disturbances in unmeasured variables.
- In case of an oscillatory disturbance : the effect of the oscillation frequency on the analysis and parameter selection.

To sum up, the findings of this study suggest that when trying to capture the causality of complex industrial systems, the application of data-based methods alone may result in numerous spurious results. Therefore, this thesis proposes a new hybrid approach for causal analysis by applying data-based methods in conjunction with the process connectivity information using a specialized search algorithm. The utilization of the connectivity information is beneficial for reducing the computational effort and enhancing the results of the analysis. Furthermore, the analysis facilitates the discrimination between direct and indirect causal interactions which is essential for capturing the process causality.

These findings have a number of practical implications regarding the selection of a causality estimator in future cases. When selecting a causality estimator one should primarily consider the system non-linearity, the type of disturbance and the computational effort involved in the implementation. This study has shown that both linear and non-linear methods are able to provide satisfactory results. Moreover, in case there is a certain level of linearity between the variables in a system, the linear methods should suffice. Therefore, a reasonable approach for causal analysis in industrial processes could be to initially apply one of the linear methods. Then, if necessary, additional non-linear methods can be applied to complement the analysis. Alternatively, several data-based methods can be applied in parallel or the system can be broken into smaller sub-systems and analyzed separately. In any case, it is important to bear in mind that process knowledge acquired from the P&ID or process experts is valuable for validating the results.

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