Self-learning Anomaly Detection in Industrial Production

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M.Sc.
Ankush Meshram

aus Brahmapuri, Indien

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Erster Gutachter: Prof. Dr.-Ing. habil. Jürgen Beyrer
Zweiter Gutachter: Prof. Dr. Veit Hagenmeyer
Abstract

Industrial production systems of the 21st Century are designed for production cost reduction through efficient control of cyber-physical industrial components. It is realized through the adaptation of Ethernet technology in industrial networking, which blurs the separation between the office networks and the industrial networks, to make a sensor in the production floor accessible to the personnel in the corporate office. The blurring of network separation led to cybersecurity vulnerabilities to industrial production, as demonstrated by recent cyber incidents from Stuxnet to Triton in the last decades. An anomaly-based Network-based Intrusion Detection Systems (NIDS) is one of the cybersecurity countermeasures that monitors the network traffic of an industrial production and learns the characteristics from its network infrastructure information to detect the deviations as anomalies. However, the network infrastructure information, such as asset inventory and security policies, are not always available for industrial productions that are non-compliant to the technological advancements in security mechanisms. In such a scenario, the configuration or designing the security countermeasures such as NIDS is challenging. An empirical solution is to self-learn the network infrastructure information (topology, assets and communication links) and the spatio-temporal behaviour from passive monitoring of industrial network traffic, in conjunction with an anomaly detection system to detect anomalies. In the absence of industrial process information, learning the process behaviour from the network traffic for anomaly detection is a challenge.

In this dissertation, solutions for the different challenges posed by the self-learning anomaly-based NIDS for industrial production are presented. For the development and evaluation of reported solutions, a miniaturized PROFINET-based industrial production system, Festo Demonstrator, developed at the
Abstract

IT-SECURITY LABORATORY, FRAUNHOFER INSTITUTE OF OPTRONICS, SYSTEM TECHNOLOGIES AND IMAGE EXPLOITATION, KARLSRUHE (IOSB) is employed. Various cyber attacks on the demonstrator are simulated and the generated network traffic is used for the evaluation. A systematic Python-based framework passively captures the network traffic from PROFINET-based system and extracts relevant information for further analysis as the solution to the challenge of making the industrial network transparent. The extracted network infrastructure information are: network topology, assets and their attributes, communication links established between master and slave (referred as PROFINET Connection), time-stamped process data payload bytes.

The industrial operations of a production system executed in an order create the foundation for process data exchanges realizing the underlying intended process. It is a challenge to enumerate and track the industrial system’s operation behaviour from the multiple protocol communications observed in the network traffic. As the solution, the extracted network infrastructure information is utilized to systematically enumerate and track the validity of PROFINET operations at different granularities of device, process data communication link and system levels via corresponding Finite State Machines (FSM) models. The implemented framework, PROFINET Operations Enumeration and Tracking (POET), utilizes the FSM models to successfully detect the network attack on the demonstrator, where an adversary attempts to change the parameters of an industrial component through valid protocol communication but invalid PROFINET operation during the process data exchange.

The industrial process behaviour is defined by the spatio-temporal characteristics of periodic, deterministic and ordered exchange of process parameters between industrial components. In a self-learning analysis approach, there are no insights into the semantics of process values being exchanged as the information on the programmed industrial process is unavailable. It puts forward the challenges of representing the extracted time-stamped process data payload bytes and learning the spatio-temporal characteristics to detect the
deviations as anomalies. Two different representations of process information, \textit{String} and \textit{Graph}, are proposed to capture the \textit{spatial} (order of the payloads) and \textit{temporal} (interval between process payload exchanges) characteristics. Consequently, two different approaches of process behaviour analysis for anomaly detection in industrial production are explored. The industrial process is conceptualized as the constituent of multiple sub-processes. Each sub-process represents the process data communication link established between a pair of master and slave devices exchanging a particular process parameter of the overall process.

In the first approach, the extracted ordered process data payloads are represented as \textit{String}, where the finite set of payload bytes are alphabet-encoded for the industrial production’s process and its constituent sub-processes. The temporal information associated with payload bytes is utilized to define the transition intervals between pair of adjacent encoded payload bytes, thus, capturing the \textit{spatio-temporal} characteristics. A systematic framework, \textit{Payload Bytes Profiling (PBP)}, represents the \textit{spatio-temporal} characteristics into spatial (\textit{transition profile}) and temporal (\textit{interval profile}) profiles. A Regular Expression-coupled Suffix Tree algorithm extracts the \textit{transition profiles} at the process and sub-process granularities from the alphabet-encoded process traffic to model the \textit{spatial} characteristics of an industrial process/sub-processes. For \textit{temporal} characteristics modeling, the transition intervals between the transitions of process payload bytes in the \textit{transition profile} of the process/sub-process are modeled through non-parametric Machine Learning (ML) models - Local Outlier Factor (LOF), Isolation Forest (IF) and One-Class Support Vector Machines (OC-SVM), and represents the \textit{temporal} characteristics as the \textit{interval profile} in PBP of a sub-process or the overall process. The PBP for the \textit{Festo Demonstrator} successfully detects the anomalies triggered by the network attack on the demonstrator, where the adversary changes the process values in a sub-process to disrupt the industrial process behaviour.

For the second approach, a \textit{Graph} representation of an industrial network, \textit{graph snapshot}, captures the \textit{spatio-temporal} characteristics of its underlying process with nodes representing the industrial components and the edges being the communication link between the components. The \textit{graph snapshot} is
created from the alphabet-encoded industrial process traffic, and the transition interval information in conjunction with transitioning payload bytes and the differences in their *Cycle Counter* values are encoded on the edges over a fixed time window on the traffic. The anisotropic Graph Neural Networks (GNN) architectures (Message Passing Neural Network (MPNN), Gated Graph Convolutional Network (GatedGCN) and Graph Transformer (GT)) are employed to learn the *spatio-temporal* characteristics of process behaviour with *graph classification* as the ML task to classify *graph snapshots* as *normal* or *anomalous*. The network attack targeting the process values of a sub-process is successfully detected by the anisotropic GNN architectures demonstrating their capability to utilize the edge features encoding the *spatio-temporal* characteristics in their learning.
Kurzfassung


In dieser Dissertation werden Lösungen für die verschiedenen Herausforderungen des selbstlernenden anomalie-basierten NIDS für die industrielle


Das Verhalten des industriellen Prozesses wird durch die räumlich-zeitlichen Merkmale des periodischen, deterministischen und geordneten Austauschs von Prozessparametern zwischen industriellen Komponenten definiert. Bei einem selbstlernenden Analyseansatz gibt es keine Einblicke in die Semantik
Kurzfassung


Kurzfassung
den Netzwerkangriff auf den Demonstrator ausgelöst werden, bei dem der Angreifer die Prozesswerte in einem Teilprozess ändert, um das Verhalten des industriellen Prozesses zu stören.

Beim zweiten Ansatz erfasst eine Graph-Darstellung eines industriellen Netzwerks, *graph snapshot*, die räumlich-zeitlichen Merkmale des zugrunde liegenden Prozesses, wobei Knoten die industriellen Komponenten und die Kan ten die Kommunikationsverbindung zwischen den Komponenten darstellen. Der *graph snapshot* wird aus dem alphabetisch kodierten industriellen Prozessverkehr erstellt, und die Übergangsintervallinformationen in Verbindung mit den übergehenden Nutzdatenbytes und den Unterschieden in ihren Cycle Counter-Werten werden an den Kanten über ein festes Zeitfenster des Verkehrs kodiert. Anisotropische Graph Neural Networks (GNN) Architekturen (Message Passing Neural Network (MPNN), Gated Graph Convolutional Network (GatedGCN) und Graph Transformer (GT)) werden verwendet, um die räumlich-zeitlichen Merkmale des Prozessverhaltens zu erlernen, wobei die ML-Aufgabe der Graphenklassifizierung die *graph snapshots* als normal oder anomal klassifiziert. Der auf die Prozesswerte eines Teilprozesses abzielende Netzwerkangriff wird von den anisotropen GNN-Architekturen erfolgreich erkannt, was ihre Fähigkeit unter Beweis stellt, die Kantenmerkmale, welche die räumlich-zeitlichen Merkmale kodieren, beim Lernen zu nutzen.
Acknowledgements

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Ankush Meshram
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1 Introduction

The fourth industrial revolution of cyber-physical systems is the consequence of incremental technological advancement since steam-powered manufacturing mechanization (the first industrial revolution) to the third industrial revolution of computer-driven process automation. Different control systems, Programmable Logic Controller (PLC), Supervisory Control and Data Acquisition systems (SCADA) and Distributed Control Systems (DCS), in different industrial sectors (chemical, power distribution, manufacturing) have been developed to efficiently achieve desired sector-specific outcomes with lower monetary cost and almost-to-none hazardous incidents. The network of interconnected equipments employed to monitor and control the industrial operations constitutes Industrial Control Systems (ICS) network or industrial network or Operational Technology (OT) network. It differs from traditional Information Technology (IT) network, or office network, in term of connectivity requirements of end users for general purpose transfer of information through Internet. However, the modern industrial communication infrastructure incorporated IT networking strategies and related protocols for shop-floor to enterprise end user access, gaining finer control on the industrial process at the cost of vulnerability to cyber threats. As a result, cybersecurity is needed to protect the industrial assets from malicious intents of the threat actors.

The modern industrial communication network can be classified in different sub-networks, as shown in fig. 1.1. Each sub-network is characterized by its role in industrial process operation, where different sub-network specific industrial components are communicating via underlying networking infrastructure.
1 Introduction

*Figure 1.1: Industrial Communication Architecture.*

**Process Control Network:** At the core of industrial operation, sensors, actuators, transmitters and I/O devices are orchestrated to realize the industrial process, and controllers such as PLCs, DCS execute the control logics of the industrial process.

**Supervisory Control Network:** Maintenance and supervision of industrial process, on-demand change of process control logic, collection and storage of process values are performed through Human-Machine Interfaces (HMI), Manufacturing Execution Systems (MES), Data Historians, Engineering and Operator Workstations.
**DeMilitarized Zone (DMZ) Network**: Following the industrial cybersecurity standards NIST SP 800-82 [Sto08] and IEC 62443 [COD13], the OT network should be separated from the IT network to limit access to process information and modification of software infrastructure in OT. Patch management servers, anti-virus servers and remote access management servers are DMZ’s constituents.

**Enterprise Network**: The corporate-level business decisions are driven through the data collected from OT networks supported through Enterprise Resource Planning (ERP), user management servers, file servers and IT related functional components. The access to Internet is restricted beyond the network. Firewalls to filter network traffic across different sub-networks are placed at the sub-network edges. Network switches are used to relay information within the sub-network, and routers for network communication across sub-networks.

Introduction of IT technology into the OT networks has started to blur distinction between office and industrial networks. However, there are fundamental differences in requirements and characteristics of office and industrial networks [Gal12], summarized in table 1.1 and expanded as follows:

**Primary Function.** Industrial networks are employed to control physical equipments which are directly affecting the physical world. On the other hand, office networks are transferring data for processing digital information such as files, audio-visual information, logistical data, etc.

**Application Domain.** Wherever there is machinery that requires monitoring and controlling, an industrial network is commissioned. The industrial domains where such a network is utilized are discrete manufacturing (automotive industry), process control (electricity generation), utility distribution (water distribution), transportation (railways) and embedded system (car’s control network). IT networks find their end users in corporate and home environments.
Table 1.1: Characteristic differences of Industrial and Office networks.

<table>
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<tr>
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<th>Industrial Networks</th>
<th>Office Networks</th>
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<tr>
<td><strong>Primary Function</strong></td>
<td>Control of physical equipment</td>
<td>Data processing and transfer</td>
</tr>
<tr>
<td><strong>Application Domain</strong></td>
<td>Manufacturing, utility distribution</td>
<td>Corporate and home environments</td>
</tr>
<tr>
<td><strong>Failure Severity</strong></td>
<td>High, industrial disasters</td>
<td>Low, information unavailable</td>
</tr>
<tr>
<td><strong>Real Time Availability</strong></td>
<td>High, response time</td>
<td>Moderate, response time</td>
</tr>
<tr>
<td><strong>Determinism</strong></td>
<td>High, low jitter</td>
<td>Low, high jitters dropped</td>
</tr>
<tr>
<td><strong>Traffic</strong></td>
<td>Periodic and aperiodic</td>
<td>Aperiodic, “best effort“</td>
</tr>
<tr>
<td><strong>Spatio-Temporal Consistency</strong></td>
<td>Required</td>
<td>Not required</td>
</tr>
<tr>
<td><strong>Network Protocols</strong></td>
<td>PROFIBUS, PROFINET,...</td>
<td>TCP/IP, UDP, FTP,...</td>
</tr>
</tbody>
</table>

**Failure Severity.** The impact of failure in industrial networks is high leading to Human, Societal and Environmental (HSE) hazards. For example, the industrial disaster of Fukushima Daiichi in 2011. When an IT network is down, the unavailability of information on a webpage or web services has relatively less severity to the industrial disaster.

**Real Time Availability.** Industrial applications such as motion control require data to be transmitted and received within the duration of $250 \mu s - 1 \ms$, and less stringent processes require $1 \ms - 10 \ms$ of response time. Office networks have moderate response time requirement of $\geq 50 \ms$.

**Determinism.** The variance in the response time of a signal is referred as jitter. Industrial networks require low jitters for real-time availability, implying data is sent and received in highly deterministic manner. Office network applications are not usually impacted by jitters. However, Voice over Internet
Protocol applications are exceptions that require low jitter, and higher jitter packets are dropped without affecting considerable its intended purpose.

**Traffic.** Process data is exchanged periodically in industrial networks, and diagnostic data (such as alarm notifications) are transmitted in an aperiodic manner. The IT networks transmit data with “best effort” delivery service.

**Spatio-Temporal Consistency.** In industrial networks, the data needs to be transmitted with temporal consistency in an ordered manner. No such guarantee is required in IT networks.

**Network Protocols.** Industrial protocols satisfying above mentioned requirements have been in development since 1980s. Serial-based fieldbus protocols such as *Process Field Bus (PROFIBUS)* and *Modbus* were developed in parallel to replace traditional two-wire signalling of control loops. Ethernet-based industrial protocols such as *Process Field Net (PROFINET)*, *Modbus Transmission Control Protocol (Modbus/TCP)* and *Ethernet Industrial Protocol (Ethernet/IP)* are the result of incorporating Ethernet technology for fast real-time industrial communication. The *Internet protocol suite* protocols (*Transmission Control Protocol (TCP)* and *Internet Protocol (IP)*, *User Datagram Protocol (UDP)* and *File Transfer Protocol (FTP)*) are some of IT protocols used for transmitting network application-specific data between end users.

### 1.1 Cybersecurity in Industrial Networks

The security objective for IT networks revolve around *confidentiality, integrity* and *availability* of information, the CIA triad. The IT protocols were developed while considering these security objectives resulting in secured protocols such as *Transport Layer Security (TLS)*, *Secure Shell Protocol (SSH)*, etc. For industrial networks, the availability of information in real-time is of the highest priority. The CIA triad didn’t suffice to the requirements of industrial network security, hence, its security objectives are categorized as basic foundational requirements in IEC 62443 [COD13]: *Access Control (AC), Use Control (UC), Data Integrity (DI), Data Confidentiality (DC), Restrict Data Flow (RDF), Timely Response to Event (TRE)* and *Resource Availability (RA).*
Table 1.2: Summary of cyber incidents targeted at industrial systems in last decades.

<table>
<thead>
<tr>
<th>Threat</th>
<th>Target</th>
<th>Exploit</th>
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<tr>
<td>STUXNET (2010)</td>
<td>Uranium enrichment facility in Iran</td>
<td>Siemens PLC to control nuclear enrichment centrifuge speed</td>
</tr>
<tr>
<td>BLACKENERGY 2 (2010)</td>
<td>Western militaries, governments, industrial sites, etc.</td>
<td>Internet connected HMI to learn industrial process and graphical representation of industrial network</td>
</tr>
<tr>
<td>Dragonfly/HAVEX (2013)</td>
<td>Multiple sectors (energy, aviation, etc.) primarily the United States and Europe</td>
<td>OPC protocol to map out industrial network</td>
</tr>
<tr>
<td>Ukraine Cyber Attack/BLACKENERGY 3 (2015)</td>
<td>Three power companies in Ukraine</td>
<td>Gained access to corporate network and pivot into SCADA networks</td>
</tr>
<tr>
<td>CRASHOVERRIDE (2016)</td>
<td>Transmission level substation in Ukraine</td>
<td>Sophisticated attack learning industrial process, leveraging OPC protocol and HMI against grid operations</td>
</tr>
<tr>
<td>TRITON (2017)</td>
<td>Petrochemical company in Saudi Arabia</td>
<td>Gained remote access to Triconex Safety controllers and entered it in failed safe state leading to automatic shutdown of the industrial process</td>
</tr>
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</table>
Fieldbus protocols were designed to make information available as quickly as possible for industrial process operations without any consideration to security of network communication. “Security by Obscurity” or “Air Gapping” defined the security policies of automation community as the communication was restricted to industrial shop-floor and never interacted with outside the industrial system’s barrier. When Ethernet technology paved its way into industrial networks, it brought along network vulnerabilities of IT systems. Exploitation of these vulnerabilities resulting in the violations of security objectives is termed as a threat or an attack. Common types of attacks are Distributed Denial-of-Service (DDoS), Man-in-the-Middle (MitM), eavesdropping, virus/trojan/worm and physically breaking into a system [Dzu05]. Advanced Persistent Threats (APT) are the highly skilled adversaries repeatedly targeting the industrial systems for espionage or malfunctioning the underlying process to cause monetary, social, environmental and personnel destructions. Some of the cyber incidents in last two decades [Lee17] are summarized in table 1.2. From the exploits of the table 1.2, it can be observed that the vulnerabilities of industrial communication network and its constituent infrastructure are being targeted to achieve adversarial goals.

A network security design principle of “Security in Depth” has been formulated as the countermeasure strategy to detect and analyse security vulnerabilities in industrial networks. At the perimeter of each layer in multi-layered industrial communication, the employed security measures isolates the subsequent layer from external threats. The outermost layer restricts the access to industrial networks to authorized personnel through Firewalls and Virtual Private Networks (VPN). DMZ tightens the security between the office and the industrial networks with shareable equipments placed in this layer to avoid direct access to industrial networks. To prevent unauthorized physical access to physical equipments, ‘hardening the equipment’ strategy is followed through password-protection on every device, blocking unused ports on switches and routers, periodic update of installed software and operating system. In order to maintain data confidentiality, integrity and authentication of the communication channels, application of cryptographic algorithms to industrial network security is the hot area of research.
As the security mechanisms for network security evolve, the older industrial equipments are mostly incapable of deploying advanced measures. To counteract the scenario, an effective security policy needs to be formulated which requires analysis of network security policies and network infrastructure, including network design and protocols, for detecting and mitigating the vulnerabilities. Intrusion Detection Systems (IDS) address all these requirements through monitoring the network to detect known attack patterns and/or deviations in the monitored behaviour of system or network.

IDS technologies can be differentiated based on the types of monitored events and analysis techniques/methodologies employed over the monitored events to detect cyber threats. The most common IDS are Host-based Intrusion Detection Systems (HIDS) and Network-based Intrusion Detection Systems (NIDS). NIDS monitors network traffic and application protocol activity in network segments. HIDS monitors characteristics and events occurring within hosts or devices on which they are deployed, such as HMI, SCADA servers and Operator/Engineering workstations. The intrusion detection methodologies can be categorized as: signature-based, anomaly-based and stateful protocol analysis. Signature-based detection compares known threat signatures to observed events through comparison operations such as string comparison. It is ineffective to multi-event attacks and unknown threats. Anomaly-based methods are effective in detecting unknown attacks using statistics, expert-knowledge and machine learning methods to compare normal activity profile against observed events to identify significant deviations. If the complex and real world activity of industrial operations are not meticulously captured, it results in high false positives. Stateful protocol analysis compares predetermined profiles based on network protocol standard against observed protocol activity to detect deviations. The analysis requires constant updating as and when protocol standard specification changes.

### 1.1.1 Anomaly Detection in Industrial Networks

Within an industrial network, the network elements and segments are connected by network switches, and firewalls deployed at the edges of segments
aid in filtering the flow of authorized traffic across. Network monitoring collects and analyses data from the network segments (network traffic) and elements (switch and firewall logs) to provide network transparency in terms of participants with their networking related properties and communication links between them. This information creates the foundation on which anomalies are detected by anomaly detection systems. It learns the network’s topology, the communication links, time-related behaviour and communication content to flag deviations as anomalies. Germany’s Federal Office for Information Security (BSI) in its cybersecurity recommendations on production networks [BSI19] outlined anomalies in industrial networks and related categories of feature requirements for anomaly detection system. The selected feature requirements of detecting the outlined anomalies in an industrial network are summarized as follows:

(1) Category A: general requirements

- overview of all devices communicating in the network,
- identification of protocols used in the network,
- identification of all the communication links in the network,

(2) Category B: unusual or exceptional activities in an ICS network

- identification of new devices in the network,
- identification of communications between two devices that was previously non-existent,
- identification of new protocols or changes in protocol among individual components,

(3) Category C: abnormal events in logs typical of production environments

- identification of ICS-specific function codes that have not previously been used,
- the ability to determine whether an access attempt (e.g. read/write) pertains to an address that is not normally used by the device at hand,
(4) Category D: unusual changes in process data (sensor data, control data, etc.)

- identification of changes in time-related behaviour,
- identification of deviations within defined value ranges

The BSI recommendation highlights the difference between “passive” and “active” solutions for network monitoring and anomaly detection. The passive system collects data passively using network or wire taps, and has no impact on data or time-sensitive behaviour of the network. An active system creates requests to network switches or devices thus generating data in the industrial network’s traffic. The system needs to be configured to ignore its own data for the analysis. In addition, the change in time-sensitive behaviour caused due to additional data transmission needs to be factored in while deploying such a system.

1.2 The Self-learning Approach

Industrial systems are commissioned for longer duration amounting to decades. The technological advancements in industrial security mechanisms are not easily deployable to non-compliant industrial network infrastructures. The industrial components can’t be always upgraded to communicate with latest industrial protocols as it is an expensive process for the plant owner. Nevertheless, it is essential to design the security of industrial network with all the available information. When access to network infrastructure information, such as asset inventory and network policies, of an existing industrial system is unavailable, designing the security policies or configuring the countermeasures such as NIDS is challenging. An empirical solution is to self-learn the network infrastructure information (topology, assets and communication links) and the spatio-temporal behaviour from passive monitoring of industrial network traffic, in conjunction with an anomaly detection system to detect anomalies. However, in the absence of industrial process information, learning the process behaviour from the network traffic for anomaly detection is a challenge.
A self-learning framework for passive network monitoring and anomaly detection in industrial networks (refer fig. 1.2) consists of following components:

1. **Data Collection**
2. **Network Information Extraction**
   - Network Topology
   - Process Data Exchange
   - Communication Links
   - Asset Attributes
3. **Network Information Representation**
4. **Network Information Analysis**

**Figure 1.2:** A Self-learning pipeline for network traffic analysis.
(a) **Data Collection and Network Information Extraction.** The unencrypted industrial network traffic is collected through network taps on wires or mirror ports on network switches. The modern industrial protocols are based on Ethernet and the data is transmitted across as series of Ethernet frames between the participants. Each frame is dissected to extract information from structured Header and unstructured Data parts for network monitoring or NIDS and process data analysis or condition monitoring, respectively, as shown in fig. 1.3. Different types of information or features can be summarized from dissected frames: flow statistics (e.g. throughput \((\text{Bytes/second})\)), protocol transactions (e.g. TCP Handshake), process values (e.g. Modbus registers), and topological information (e.g. sender and receiver Media Access Control (MAC) addresses).

(b) **Network Information Representation.** The representation of extracted network information depends on the requirements of the analysis method. NetFlow was introduced by Cisco to represent network flow information capturing ingress and outgress quantitative features such as network throughput rate \((\text{Bytes/second})\). String-based representation is the staple for n-gram analysis methods [Wre13] and other string-based intrusion detection methods such as ZOE [Wre18]. Graph representation have been used for graph-based analysis methods such as GNN [Bus21, Puj21]. The network information can
be represented as images or bitmaps for image analysis based intrusion detection methods [Kim05]. There are also proprietary representation used by respective methodologies such as nPrint [Hol21] and Zeek/Bro [Pax99].

Figure 1.4: Summary of Anomaly-based Intrusion Detection System methodologies [Hin18].

(c) Network Information Analysis. After network information is represented in an analysis method’s required format, it forms the basis for learning the network’s assets, communication links, time-based behaviour and process communication. The deviations from the learnt behaviour are reported as
1 Introduction

anomalies. Hindy et. al. [Hin18] have summarized the different categories of anomaly-based intrusion detection techniques as statistical, knowledge-based and ML-based, shown in fig. 1.4. Univariate models, multivariate models and time-series analysis are employed as statistical methods for anomaly-detection. For knowledge-based anomaly detection, finite state machines, description languages, expert systems, n-grams and rule-based methods are grouped together in this category. ML-based techniques encompasses data mining methods along with neural networks, deep learning methods, support vector machines, decision trees, bayesian networks, markov models, genetic algorithms, etc.

1.3 Research Objectives and Contributions

An industrial system’s behaviour consists of two components: (a) the networking operations beginning at the start-up of the system until the process data exchange begins, and (b) the periodic and deterministic industrial process. The network information representing the two aspects of an industrial system’s behaviour are embedded in the multiple protocols communicating over the networking infrastructure. One or multiple protocols are employed at different stages of the networking operations to configure the network assets for process data exchange.

To self-learn an industrial system’s behaviour from network traffic, the network information needs to be systematically extracted while enumerating the networking operations. After the network is made transparent for downstream analysis, the system behaviour needs to be learnt from the extracted information for anomaly detection. The research questions that arises to self-learn an industrial system’s behaviour from the passively monitored network traffic and the empirical solutions developed to answer the research objectives are summarized in this section.

In the quest for finding the solutions to research questions, a PROFINET based industrial system is used for developing and evaluating the proposed solutions. PROFINET has 18% market share in the industrial networks that are
installed globally in 2021 as compared to 17% *EtherNet/IP* [NID21]. Additionally, *PROFINET* is the leader of Industrial Ethernet technology in the European market which concluded its selection as the industrial system under consideration for the presented work. A *PROFINET*-based scaled-down industrial system with real industrial components and fully functional networking infrastructure, labelled as *Festo Demonstrator*, developed at IT-SECURITY LABORATORY, FRAUNHOFER IOSB [Pfr16, 20] is employed for the reported analysis. The network attacks targeted at the *Festo Demonstrator*’s underlying network and process operations are scripted, executed and resulting anomalies are passively captured from the network traffic. The details of the demonstrator and network attack scenarios are provided in section 2.5.

### 1.3.1 Industrial Network Transparency

The networking operations such as neighbourhood detection and connection establishment that an industrial communication network undergoes, contains all the required information for network monitoring. The industrial network’s topology, communication relations, assets and protocol data being exchanged during the industrial process operation are the network information to be extracted from the network traffic passively. For extracting the network information in a self-learning scenario, detecting the different industrial operations from start-up to process data exchange from the network traffic in a systematic way is required and defines the research objective for network transparency.

**Research Question 1:** *How to extract information of an industrial system from its network traffic?*

An industrial system’s process is conceptualized and engineered outside the networking operations in an engineering tool. The devices are configured as per the requirements of process and the process control logic is loaded onto the controllers. As soon as the system starts up, the devices are communicating with each other to establish their neighbours in the vicinity and communication links between master devices and their corresponding slave devices. In chapter 3, different industrial networking operations are mapped to their
industrial operation counterparts. PROFINET’s specifications are followed to correctly map network protocols to detect networking operations and their constituent stages. For this, the Python-based Scapy framework [Bio22] is utilized to dissect network packets in order to extract relevant information for detecting networking operations and populate different network information: network topology, assets and their attributes, communication links established between master and slave (referred as PROFINET Connection), time-stamped process data payload bytes.

**Contribution 1:** A Python-based framework that passively captures the network traffic from PROFINET-based system and extracts relevant information to make the industrial network transparent for analysis.

### 1.3.2 Industrial Operations Behaviour

The industrial operations executed in an order create the foundation for process data exchanges realizing the underlying intended process. Enumerating these operations through the analysis of multiple protocol communications observed in the traffic and tracking their executions helps to define the industrial system’s operation behaviour. Addition of a device to the network and device’s attempt to establish communication for process data exchange triggers execution of network operations. Monitoring the valid operations of devices, communication links or the industrial system would detect the adversarial actions in the context of employed Industrial Ethernet technology’s network protocol communication specifications. The research objectives for self-learning an industrial system’s operation behaviour are: (a) selecting the appropriate network information extracted from network frames for operation enumeration, (b) representing the executions of operations and their constituent stages to learn the operation’s behaviour, and (c) selection or development of an analysis method to detect deviations.

**Research Question 2:** How to enumerate and track an industrial system’s operations from network traffic?
In chapter 3, the network information made available through the developed network transparency solution are utilized to enumerate different industrial operations whenever they occur. An industrial system’s operation behaviour is considered at device-level, connection-level and system-level to track operational state changes in devices, established process exchange communication links and the overall system. *Finite State Machines (FSM)* are conceptualized for each device, connection and industrial system, where nodes represent the stages of industrial operations and the edges are the transitions that are triggered by the events observed in the extracted network information from the traffic. The self-learning methodology is summarized in table 1.3. A *Python*-based framework that extracts the network information from *PROFINET*-based industrial system’s network traffic to instantiated appropriate FSM models (Device, Connection or System) and track the industrial operations is developed as *PROFINET Operations Enumeration and Tracking (POET)*. In section 3.5.1, POET is employed to detect anomalies triggered by a network attack targeted at *Festo Demonstrator’s* device *Turntable-Motor*. The attack is executed through valid *PROFINET Discovery and Configuration Protocol (PN-DCP)* exchanges, resulting in invalid *PROFINET* operation transition for the device leading to successful detection and reporting by POET.

**Contribution 2:** Graph-represented Finite State Machine models for valid industrial operations and their transitions at device-level, connection-level and system-level.

**Contribution 3:** *PROFINET* Operations Enumeration and Tracking (POET) as a framework to enumerate *PROFINET* operations from the events embedded in network information and track the operation transitions to report invalid transitions as anomaly, acting as a Protocol-analysis based Network-based Intrusion Detection Systems (NIDS) for *PROFINET*. 

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Table 1.3: Summary of proposed behavioural analysis methods.

<table>
<thead>
<tr>
<th></th>
<th>Extracted Network Information</th>
<th>Network Information Representation</th>
<th>Network Information Analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Industrial</strong></td>
<td><strong>Network Topology</strong></td>
<td><strong>Finite State Machines for PROFINET operations (section 3.4)</strong></td>
<td><strong>Finite State Machines</strong></td>
</tr>
<tr>
<td>Operations</td>
<td><strong>Asset and attributes</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Behaviour</strong></td>
<td><strong>PROFINET Connection</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Spatio-temporal</strong></td>
<td><strong>Time-stamped Process</strong></td>
<td><strong>String-represented Process</strong></td>
<td><strong>- Regular Expressions-coupled</strong></td>
</tr>
<tr>
<td><strong>Process</strong></td>
<td><strong>Data Payload Bytes</strong></td>
<td><strong>Payload Byte Profiles</strong></td>
<td><strong>Suffix Tree (section 4.3)</strong></td>
</tr>
<tr>
<td><strong>Behaviour</strong></td>
<td></td>
<td></td>
<td><strong>- Machine Learning</strong></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>models: LOF, IF, OC-SVM</strong></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>(section 4.4)</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Graph-represented</strong></td>
<td></td>
<td><strong>Anisotropic Graph Neural Networks:</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Graph Snapshots</strong></td>
<td></td>
<td><strong>MPNN, GatedGCN, GT</strong></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>(section 5.5)</strong></td>
</tr>
</tbody>
</table>
1.3.3 Industrial Process Behaviour

The industrial process behaviour is defined by the periodic, deterministic and ordered exchange of process parameters between industrial components. The *spatio-temporal* characteristics of the process data exchange represents the industrial process behaviour, where a finite set of process values are exchanged in a redundant manner. An adversary with access to the information on underlying industrial process of an industrial system could tamper either the process parameter values or delay the network frames to exploit the data integrity (DI), time to response (TRE) and resource availability (RA) security objectives of the industrial system. In a self-learning analysis approach, there are no insights into the semantics of process values being exchanged as the information on the programmed industrial process is unavailable. However, the *spatio-temporal* characteristics of finite set of payload bytes extracted from the process data frames are representative of embedded process values. The representation of payload bytes with temporal information of their occurrences to learn the *spatio-temporal* characteristics and detecting their deviations as anomalies are the research objectives for self-learning an industrial system’s process behaviour.

**Research Question 3:** How to represent the *spatio-temporal* characteristics of an industrial system’s process?

**Research Question 4:** How to learn the *spatio-temporal* characteristics of an industrial system’s process for anomaly detection from the network traffic?

The industrial process is expressed as the constituent sub-processes of an industrial system. A sub-process represents the process data communication link (Connection) established between a pair of master and slave devices exchanging a particular process parameter of the overall process. The overall interplay of different process parameter exchanges in the constituent sub-processes drives the industrial process. With the coarse and fine granular perspectives of an industrial process, in this thesis two different representations for the *spatio-temporal* characteristics and related process data analysis methodologies have been proposed in chapter 4 and chapter 5, summarized in table 1.3.
In chapter 4, the ordered process data payload bytes are represented as a *String*, where the finite set of payload byte strings of every sub-process are encoded as alphabets. The alphabet-encoded payload bytes, when sequentially arranged, define the encoded network traffic and every pair of adjacent alphabet-encoded payload bytes defines a transition. The temporal information associated with process payload bytes is utilized to define the transition intervals for each transition observed.

A *Python*-based framework called *Payload Bytes Profiling (PBP)* extracts the process data payload bytes, encodes them in alphabets and profiles the *spatio-temporal* characteristics for sub-processes and the industrial process is developed as the empirical solution. The *transition profile* of PBP captures the finite set of alphabet-encoded payload bytes representing the production cycle which is extracted using Regular Expression-coupled Suffix Tree algorithm, refer section 4.3. The transition intervals for each transition pair in the transition profile is modeled using non-parametric Machine Learning (ML) models Local Outlier Factor (LOF), Isolation Forest (IF) and One-Class Support Vector Machines (OC-SVM), and stored as the *interval profile* in PBP of a sub-process or the overall process, refer section 4.4. The combination of *transition* and *interval profiles* in a PBP of a sub-process/process models the *spatio-temporal* characteristics and detects the deviations as anomalies, refer section 4.4.3 The PBP framework successfully detected the anomalies triggered by changing the process values in *Festo Demonstrator*’s sub-process to move the *Lower Belt* device in opposite direction, refer section 4.6.2. In addition to anomaly detection, the production cycle of *Festo Demonstrator*’s industrial process is successfully detected through its transition profile extraction from the encoded traffic using PBP framework, refer section 4.6.1.

**Contribution 4:** Payload Bytes Profiling (PBP) as a systematic framework to represent the *spatio-temporal* characteristics of an industrial system’s process and its constituent sub-processes as spatial (*transition profile*) and temporal (*interval profile*) profiles from passively monitored network traffic.

**Contribution 5:** A methodology to extract the periodic process data exchange at process and sub-process granularity with Regular Expression-coupled Suffix Tree algorithm from *String* represented network traffic.
1.3 Research Objectives and Contributions

**Contribution 6:** A methodology based on non-parametric Machine Learning (ML) models (Local Outlier Factor, Isolation Forest and One-Class Support Vector Machines) to capture intervals between process payload bytes as the *temporal* characteristic of an industrial system’s sub-process/process.

In chapter 5, the ubiquitous *Graph* representation of an industrial network to learn the *spatio-temporal* characteristics of the underlying industrial process is proposed. The graph structure represents the network topology with *nodes* being the industrial components and the *edges* being the communication link between the components. Especially, for capturing the process behaviour in the graph, the edge represents the communication link established for process data exchange. The network traffic encoding scheme from chapter 4 is utilized to represent the process data exchanges as a string of alphabet-encoded process payload bytes with temporal information. In addition to the transition interval, the differences in the *Cycle Counter* values of transitioning payloads is utilized to capture the network behaviour extracted from the *structured Header* part of network frames. To represent the *spatio-temporal* characteristics of industrial process, a *graph snapshot* over a fixed time window on the traffic is utilized, refer section 5.4. For each sub-process represented by the edge of the graph snapshot, the payload byte transitions along with interval and cycle counter differences are binary encoded.

In order to learn the *spatio-temporal* characteristics represented in graph snapshots, Graph Neural Networks (GNN) models are employed to compute embeddings for the nodes, edges and overall graph for downstream ML tasks such as *node/edge/graph classification, link prediction*, etc., refer section 5.3. Three different anisotropic GNN architectures (Message Passing Neural Network (MPNN), Gated Graph Convolutional Network (GatedGCN) and Graph Transformer (GT)) are evaluated for learning the process behaviour from the graph snapshots and anomaly detection is modeled as the *graph classification* task to classify each graph snapshot as *normal* or *anomalous*. An isotropic GNN, Graph Convolutional Network (GCN), is used as the baseline, refer section 5.5. The learnt GNN architectures are employed to detect anomalies in the process traffic, triggered by changing the process values in *Festo Demonstrator’s* sub-process to move the *Lower Belt* device.
in opposite direction. The anisotropic GNNs are successful in detecting the anomalies in comparison to isotropic GNN architecture.

**Contribution 7:** A *Graph* representation of an industrial system’s *spatio-temporal* characteristic process as *graph snapshots* over the passively monitored network traffic.

**Contribution 8:** Demonstration of anisotropic Graph Neural Networks (GNN) architecture usage to learn the process behaviour with *graph classification* as the ML task to classify *graph snapshots* as *normal* or *anomalous*.

### 1.4 Thesis Outline

In *Chapter 2*, a brief introduction to industrial communication protocols, cyber threats in industrial networks, IDS taxonomy for industrial networks and publicly available datasets for industrial cybersecurity are sketched. The description of *Festo Demonstrator* and implemented attack scenarios are also provided.

*Chapter 3* details the networking operations of a *PROFINET*-based industrial production system detected from its network traffic to populate the network infrastructure information and make the industrial network transparent for further analysis. The *POET* framework that enumerates and tracks the *PROFINET* operations using different Finite State Machine models at different granularities and its usage for anomaly detection are outlined.

In *Chapter 4*, the self-learning approach for process behaviour analysis based on *String* representation of the process data extracted from the network traffic is presented. The details of *PBP* framework with *spatial* and *temporal* characteristic modeling methods for anomaly detection are described.

*Chapter 5* describes the usage of anisotropic GNN architectures to self-learn the *spatio-temporal* characteristics of an industrial process which is graphically represented as *graph snapshots*. The *graph snapshots* are classified as either *normal* or *anomalous*.
In *Chapter 6*, the contributions of the dissertation ensued from the reported solutions to the research questions with discussion and an outlook to improve the solutions are provided.
2 Preliminaries

In this chapter, the foundational information required for the reported research work are provided.

2.1 Industrial Communication Protocols

In 1970s, the introduction of new technologies such as programmable micro-controllers and digital signal processors led to the replacement of traditional two-wire signalling technique for analogue control loops between connected industrial equipments with digital controllers. The International Standards Organisation (ISO) created the seven layered communication model Open System Interconnection (OSI), which facilitated creation of multiple communication protocols and services. As per the different communication characteristic requirements, the standard OSI reference model is reduced to protocol stacks: TCP/IP stack, and Manufacturing Automation Protocol/Enhanced Performance Architecture (MAP/EPA) stack, refer fig. 2.1. The reduction is driven by the real-time availability and deterministic communication requirement of industrial network communication. The reduced protocol stacks reduced the time delays incurred due to passing of information between layers and its processing at each layer [Gal12].

Serial-based fieldbus protocols built on the MAP/EPA model replaced expensive point-to-point cabling of devices to a central control room, and brought at forefront the concepts of decentralization, modularity of industrial systems and communication between intelligent devices for process and diagnostic information exchange. PROFIBUS, Controller Area Network (CAN) and Foundation Fieldbus (FF) are some of the earliest fieldbus protocols which were
independently developed in parallel for automation. The *International Electrotechnical Commission (IEC)* and *Instrumentation Society of America (ISA)* organizations jointly defined a standard for fieldbus protocols IEC 61158 to standardize independent fieldbus developments.

![Network Communication Models](image)

*Figure 2.1: An overview of network communication models.*

The incorporation of Ethernet technology into industrial networking introduced Ethernet-based industrial communication protocols. Fast data transfer rates of Ethernet accelerated *Real-Time Ethernet (RTE)* protocols for time-critical industrial applications such as motion controls. Ethernet also introduced switched networks to replace older hub based networks for efficient and error-less data retransmission in the industrial automation domain. *PROFINET, EtherCAT, EtherNet/IP, Modbus/TCP* are some of the RTE industrial protocols within the IEC 61784 standard for the Industrial Ethernet protocols.

Different application domains such as factory automation and motion controls have different real-time requirements which need different implementations
of the *TCP/IP* protocol stack to achieve the determinism. These different RTE implementations, refer fig. 2.2, are categorized based on transmission time [Dec05, Dan14] as follows:

**On top of TCP/IP.** Human centric systems such as process monitoring and engineering systems need network data transmission time around 100\,ms for observation. The *application layer* is responsible for scheduling communication to meet the requirements. This allows communication outside the network boundaries with remote devices incurring non-deterministic delays. The scheduling devices need to be equipped with adequate resources to handle the delays. Industrial protocols *Modbus/TCP* and *EtherNet/IP* are based on this RTE implementation.

**On top of Ethernet.** For process control systems, the timing requirements are below 10\,ms. Modifications at the *application layer* to use standard packets and at the *transport layer* to use custom ethertypes for real-time communication is performed. The network devices must have the knowledge of custom protocols to prioritize the custom ethertypes within the network. Within the
RTE implementation, *Ethernet Powerlink* and *PROFINET Real-Time (RT)* are the widely popular protocols.

**Modified Ethernet.** Motion control applications require a cycle time $< 1 \text{ms}$, which can be achieved only when the *data link layer* is modified to apply mechanisms and infrastructure to allow real-time communication. Customized hardware with switching functionality is employed to achieve highly deterministic timing requirements. *PROFINET Isochronous Real-Time (IRT)*, *EtherCAT* and *Serial Real-time Communication System (SERCOS)* are the Industrial Ethernet protocols based on the RTE implementation.

*Time Sensitive Networking (TSN)* is a set of IEEE 802 standards [21d] to make Ethernet deterministic by design. It aims to develop mechanisms that guarantee determinism and bounded latency in high throughput networks operating at $10 \text{Mbps}$, $100 \text{Mbps}$, $1 \text{Gbps}$ or $10 \text{Gbps}$. It offers real-time capability in industrial networks with gigabit Ethernet which is restricted in IEC 61784 Industrial Ethernet protocols. The TSN standards offer specifications for *Frame Preemption* (IEEE 802.1Qbu), *Scheduled Traffic* (IEEE 802.1Qbv), *Ingress Policing* (IEEE 802.1Qci), *Seamless Redundancy* (IEEE 802.1CB), *Time Synchronization* (IEEE 802.1AS), *Stream Reservation* (IEEE 802.1Qcc) and many more [Bra21, 21d]. The existing Industrial Ethernet protocols such as *PROFINET* and *EtherCAT* are incorporating TSN in their protocol stacks to support TSN technology for real-time networking [21c, 21b].

The *Open Platform Communications Unified Architecture (OPC UA)* framework merged with TSN, referred as *OPC UA TSN*, is the next-generation solution to integrated communication and data infrastructure requirement for seamless merging of IT and OT applications in real-time [Tri21, Hum22]. The OPC UA PubSub communication model introduced by the OPC Foundation in IEC 62641-14 builds the foundation for secure communication across devices in field level to MES/ERP and further into the Cloud. Using TSN as the communication protocol at *OSI layer 2*, the real-time deterministic control behaviour can be achieved. The TSN-enabled Switches are already available and realizing the benefits of TSN. Different automation manufacturers have began to integrate *OPC UA TSN* into their product portfolios such as *PROFINET@TSN* and *Sercos over TSN*.
### 2.2 Cyber Threats in Industrial Networks

<table>
<thead>
<tr>
<th>Initial Access</th>
<th>Execution</th>
<th>Persistence</th>
<th>Privilege Escalation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drive-by Compromise (DbC)</td>
<td>Change Operating Mode (COM)</td>
<td>Modify Program (MPgm)</td>
<td>Exploitation for Privilege Escalation (EPE)</td>
</tr>
<tr>
<td>Exploit Public-Facing Application (EPFA)</td>
<td>Command-Line Interface (CLI)</td>
<td>Module Firmware (MF)</td>
<td>Hooking (H)</td>
</tr>
<tr>
<td>Exploitation of Remote Services (EoRS)</td>
<td>Execution through API (EtA)</td>
<td>Project File Infection (PFI)</td>
<td></td>
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<tr>
<td>External Remote Services (ERS)</td>
<td>Graphical User Interface (GUI)</td>
<td>System Firmware (SF)</td>
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</tr>
<tr>
<td>Internet Accessible Device (IAD)</td>
<td>Hooking (H)</td>
<td>Valid Accounts (VA)</td>
<td></td>
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<tr>
<td>Remote Services (RS)</td>
<td>Modify Controller Tasking (MCT)</td>
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<td></td>
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<tr>
<td>Replication Through Removable Media (RTRM)</td>
<td>Native API (NA)</td>
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<tr>
<td>Rogue Master (RM)</td>
<td>Scripting (S)</td>
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<td>Spearphishing Attachment (SA)</td>
<td>User Execution (UE)</td>
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<tr>
<td>Supply Chain Compromise (SCC)</td>
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<td>Transient Cyber Asset (TCA)</td>
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<tr>
<td>Wireless Compromise (WC)</td>
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</table>

**Figure 2.3:** The MITRE ATT&CK for ICS Matrix. (Part 1)

MITRE ATT&CK for Industrial Control Systems (ICS) [Ale20] is a knowledge base of cyber adversary behaviours targeted at the ICS technology domain and it categorizes adversary’s attack life cycle into phases with targeted assets and systems. It describes an adversary’s tactical objective for performing an action, the tactical actions and instances of adversary’s techniques as the tactics, techniques and procedures (TTP). The relationships between tactics and techniques are organized in the ATT&CK Matrix, as shown in fig. 2.3 - fig. 2.5. As of February 2022, there are 78 techniques categorized into 12 tactics in ATT&CK for ICS. The adversary’s tactics are categorized in the order of attack life cycle phases as Initial Access, Execution, Persistence, Privilege Escalation, Evasion, Discovery, Lateral Movement, Collection, Command and Control, Inhibit Response Function, Impair Process Control and Impact.
An attack sequence of real threat groups usually contains multiple techniques where the attacker moves from left (Initial Access, ...) to right (..., Impact) in the ATT&CK Matrix. The table 2.1 summarizes the MITRE techniques employed by the threat groups that executed APTs Stuxnet [22d], Industroyer [22a] and Triton [22e]. The initial stages of these APTs involves IT infrastructure which is expressed in the ATT&CK for Enterprise knowledge base [Str18]. As the adversary’s targets and actions differ significantly between the Enterprise and ICS technology domains, MITRE adopted the separation of ATT&CK methodology and consequently introduced the different knowledge bases.

<table>
<thead>
<tr>
<th>Evasion</th>
<th>Discovery</th>
<th>Lateral Movement</th>
<th>Collection</th>
</tr>
</thead>
<tbody>
<tr>
<td>Change Operating Mode (COM)</td>
<td>Network Connection Enumeration (NCE)</td>
<td>Default Credentials (DC)</td>
<td>Automated Collection (AC)</td>
</tr>
<tr>
<td>Exploitation for Evasion (EFE)</td>
<td>Network Sniffing (NS)</td>
<td>Exploitation of Remote Services (EoRS)</td>
<td>Data from Information Repositories (DIR)</td>
</tr>
<tr>
<td>Indicator Removal on Host (IRoH)</td>
<td>Remote System Discovery (RSD)</td>
<td>Lateral Tool Transfer (LTT)</td>
<td>Detect Operating Mode (DOM)</td>
</tr>
<tr>
<td>Masquerading (M)</td>
<td>Remote System Information Discovery (RSID)</td>
<td>Program Download (PD)</td>
<td>I/O Image (I)</td>
</tr>
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<td>Rootkit (R)</td>
<td>Wireless Sniffing (WS)</td>
<td>Remote Services (RS)</td>
<td>Man in the Middle (MitM)</td>
</tr>
<tr>
<td>Spoof Reporting Message (SRM)</td>
<td></td>
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<td></td>
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</tbody>
</table>

**Figure 2.4**: The MITRE ATT&CK for ICS Matrix. (Part 2)
The realization of all the MITRE ATT&CK techniques in a testbed is not possible given the domain, protocol characteristics and resource availability constraints of the testbed. For the reported research and the testbed employed, procedures for Modify Parameter (MPrm) and Denial of Service (DoS) are implemented (section 2.5.3) and utilized for the development and evaluation of self-learning anomaly detection systems.

Figure 2.5: The MITRE ATT&CK for ICS Matrix. (Part 3)
<table>
<thead>
<tr>
<th>Tactic</th>
<th>Techniques Employed by APTs</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Stuxnet</td>
</tr>
<tr>
<td>Initial Access</td>
<td>EoRS, RTRM, RS</td>
</tr>
<tr>
<td>Execution</td>
<td>EtA, H, MCT, NA,UE,CLI</td>
</tr>
<tr>
<td>Persistence</td>
<td>MPgm,PFI</td>
</tr>
<tr>
<td>Privilege</td>
<td>–</td>
</tr>
<tr>
<td>Escalation</td>
<td>–</td>
</tr>
<tr>
<td>Evasion</td>
<td>M, R</td>
</tr>
<tr>
<td>Discovery</td>
<td>NS, RSID</td>
</tr>
<tr>
<td>Lateral Movement</td>
<td>DC, PD, LTT</td>
</tr>
<tr>
<td>Collection</td>
<td>II, MPS</td>
</tr>
<tr>
<td>Command and Control</td>
<td>CUP, SALP</td>
</tr>
<tr>
<td>Inhibit Response Function</td>
<td>MII</td>
</tr>
<tr>
<td>Impair Process Control</td>
<td>MPrm, UCM</td>
</tr>
</tbody>
</table>
2.3 Intrusion Detection System (IDS) Taxonomy for Industrial Networks

Hu et al. [Hu18] defines IDS for industrial networks or ICS (ICS IDS) as “devices or software applications or their combinations monitoring the behaviors of ICS for detecting malicious activities or policy violations by collecting and analyzing all available data (e.g. protocol specifications, system logs, host data, network traffics, sensor measurements, together with the domain-specific knowledge of industrial control)”. They contend that the traditional IDS taxonomy is designed for information systems and do not pay attention to peculiarity of ICS domain on its close relationship with the physical world. Hence, a new ICS IDS taxonomy is proposed based on the detection techniques and ICS characteristics as three categories: protocol analysis-based, checks protocol specification violations in an industrial control network; traffic mining-based, analyses non-linear and complex relationships between the network traffic and the normal/abnormal system behaviour, and control process analysis-based, detects semantic attacks tampering with industrial process data or operating rules of specific control systems.

![ICS IDS Taxonomy](image)

**Figure 2.6:** Hu et al.’s IDS Taxonomy for ICS/Industrial Networks [Hu18].

**Protocol analysis-based IDS.** The industrial protocols were designed with the goal of reliability and efficiency of ICS without any consideration to the cybersecurity aspects. The lack of encryption and authentication mechanisms make them vulnerable to cyber threats, and led to the emergence of protocol analysis-based IDS. A protocol specification defines the message format and
the networking operations allowed by the protocol. A protocol analysis-based
IDS uses the specifications of a protocol to detect its violation in message for-
mats and/or their exchanges to identify the abnormal behaviours in industrial communication network of ICS. Cheung et al.’s Modbus/TCP based IDS
[Che07], Snort-based IDS for Modbus by Morris et al. [Mor12], Lin et al.’s Bro-
based IDS for DNP3 protocol [Lin13a] and Hong et al.’s IDS for IEC 61850
standard protocols [Hon14] are some of the reported work in the literature
for this category of ICS IDS.

Traffic mining-based IDS. The traffic data is collected from different re-
gions in ICS and data mining or data analysis methods are applied to detect
anomalous behaviours in the network communication of ICS. Usage of Princip-
al Component Analysis (PCA) by Hou et al. [Hou12], Neural Networks (NN)
by Ashfaq et al. [Ash17], One-Class Support Vector Machines (OC-SVM) by
Maglaras et al. [Mag14], Caselli et al.’s Discrete-Time Markov Chain (DTMC)
model [Cas15] and Ant Colony based IDS by Aghdam et al. [Agh16] are some
of the reported work for traffic mining-based IDS.

Control process analysis-based IDS. The semantic information and pecu-
liarity of ICS hasn’t been considered by the traditional IDS system. A control
process analysis-based IDS includes process data analysis-based, control com-
mand analysis-based and ICS physical model-based intrusion detection tech-
niques. Hadžiosmanović et al.’s IDS based on semantic analysis of process
variables [Had14], Kiss et al.’s Gaussian Mixture Model (GMM) dependent
IDS [Kis15] and Gao et al.’s NN-based behavioural model [Gao10] are some
of the published process data analysis-based IDS. Carcano et al.’s IDS for Mod-
bus control command [Car09] and Lin et al.’s semantic analysis technique for
control commands in distributed ICS [Lin13b] are examples of control com-
mand analysis-based IDS. The linear state-space model for ICS by Cárdenas
et al. [Cár11], Myers et al.’s process mining based IDS and intrusion detection
and mitigation mechanism for smart grids reported by Sridhar et al. [Sri14]
are few examples of ICS physical model-based IDS.
2.4 Datasets for Industrial Cybersecurity

The quality and characteristics of datasets employed in the development of ICS cyber threat detection methods play an important role in driving the Industrial Cybersecurity research. Sommer and Paxson in their seminal paper on application of Machine Learning to network security [Som10] highlighted the importance of dataset quality, “an anomaly detection system that strives to find novel attacks using only simulated activity will often lack any plausible degree of realism or relevance”. In the light of this observation, different publicly available ICS datasets used by the reported Industrial Cybersecurity research in the literature are analysed and compared for different characteristics: ICS testbed class, ICS domain, ICS protocol coverage, data type and ICS threats coverage.

The datasets are classified according to the taxonomy introduced by Holm et al. [Hol15]. This taxonomy differentiates between Physical, testbeds only using real hardware and software; Software, testbeds based on software simulation and emulation; Semi-Physical, testbeds composed of real and simulated components, and Virtualized, testbeds based on the virtualization technology. The ICS domain related to each dataset is classified based on the categories defined by Teumim [Teu10]. The format and type of the data provided by the datasets defines the extent of features used for the analysis algorithms. Sommer and Paxson [Som10] highlighted this as a common pitfall in developing network intrusion detection methods, “the temptation to base the feature set on the dataset that happens to be at hand for evaluation”. The network data are provided either in already dissected (Dissected) or raw form (PCAP). In some cases, the datasets focus exclusively on process data (Process Values). The ICS network protocols used for generating the dataset are also extracted for the analysis. The attack behaviour from the datasets are analysed and categorized according to MITRE ATT&CK for ICS knowledge base for qualitative evaluation of ICS threats coverage.
Table 2.2: Comparison of public ICS datasets.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Testbed Class</th>
<th>Domain</th>
<th>Data Provided</th>
<th>Protocol Coverage</th>
<th>Technique Coverage</th>
</tr>
</thead>
<tbody>
<tr>
<td>SWaT [Mat16]</td>
<td>Physical</td>
<td>Water Supply</td>
<td>Process Values</td>
<td>EtherNet/IP</td>
<td>MPrm</td>
</tr>
<tr>
<td>GAS Pipeline [Mor14]</td>
<td>Physical</td>
<td>Gas Oil</td>
<td>Dissected, Process</td>
<td>Modbus</td>
<td>MPrm, UCM, SRM,</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Values</td>
<td></td>
<td>DRS, COM, DoS,</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>RSD, NCE</td>
</tr>
<tr>
<td>TEP Simulation [Rie17]</td>
<td>Semi-physical</td>
<td>Chemical Industry</td>
<td>Process Values</td>
<td>Not Available</td>
<td>Not Available</td>
</tr>
<tr>
<td>CSET Modbus [Lem16]</td>
<td>Software</td>
<td>Electric Power</td>
<td>PCAP</td>
<td>Modbus</td>
<td>ERS, PTI, UCM,</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>CUP</td>
</tr>
</tbody>
</table>

**Techniques:** CUP - Commonly Used Port; DoS - Denial of Service; DRS - Device Restart/Shutdown; ERS - External Remote Services; MPrm - Modify Parameter; NCE - Network Connection Enumeration; PTI - Point & Tag Identification; RSD - Remote System Discovery; SRM - Spoof Reporting Message; UCM - Unauthorized Command Message; COM - Change Operating Mode
The table 2.2 summarizes the analysis of publicly available datasets: iTrust SUTD’s Secure Water Treatment (SWaT) [Mat16] and Water Distribution (WADI) [Ahm17]; Morris et al.’s Gas Pipeline dataset (Gas Pipeline) [Mor14]; Tennessee Eastman Process Simulation dataset (TEP Simulation) from Rieth et al. [Rie17] and Modbus Dataset from CSET 2016 (CSET Modbus) from Lemay et al. [Lem16].

It can be observed from the table that there is lack of PROFINET based dataset availability which made any of these publicly available datasets not feasible for the reported PROFINET-based Industrial Cybersecurity analysis. Hence, a PROFINET-based miniaturized physical industrial process realized at the IT-SECURITY LABORATORY is employed to generate the dataset for the analysis.

### 2.5 System under Consideration

The IT-SECURITY LABORATORY, FRAUNHOFER IOSB offers a platform for industrial cybersecurity research and educational trainings. Different miniaturized manufacturing/production processes are realized as real-world demonstrators with extended virtualized infrastructure. The industrial network vulnerabilities in communication protocols or industrial components are exploited to develop threat detection methods and countermeasures for secure and safe process control communication. In particular, the datasets collected from demonstrators are real-world, encapsulating process and network communication with subtleties that can’t be emulated completely by emulators/simulators. Different threat models attacking ICS are simulated through attack scripts and executed on the demonstrators to capture their effects in network traffic for downstream analyses.
A miniaturized manufacturing process is realized on a demonstrator labelled as the *Festo Demonstrator*, shown in fig. 2.7. In the figure, the red-coloured outlined box A shows the field level with real-world automation components where the scenario process is realized. The process is controlled by real-world ICS components such as PLC and HMI, highlighted in blue-coloured outlined box B. MES with overview on execution of controlled process can be visualized on a *Tablet* in the top-left corner of B. The attack scripts simulating an attacker/adversary exploiting industrial network vulnerabilities are executed on the laptop in green-coloured outlined box C.
2.5 System under Consideration

2.5.1 Industrial Process Scenario

The process scenario realized in the Festo Demonstrator is a simplified painting process, shown in fig. 2.8. The workpieces are stored in a vertical cylinder-shaped (open at both ends) Stock. The process begins when pneumatic Piston at the bottom of Stock pushes a workpiece onto the Storage, a cylindrical turntable with 8 workpiece positions (1). In the next process step, a pneumatically operated Gripper picks up the workpiece from the Storage and places it onto the upper conveyor Belt (2). The upper Belt moves the workpiece to Sorting/Inspection system. It is inspected for defects and quality control checks. If it is defective, the Barrier opens up and it is moved to Rejects bin (3), otherwise the Barrier diverts it to slide onto lower conveyor Belt for further processing (4). On the lower Belt, the workpiece follows through Milling and Painting, and is transported to Lift’s platform at the end of the Belt (5) for drying. At the end of the Lift, a final quality control of workpiece takes place. The painting
process of workpiece ends and the pneumatic Piston at the top of Stock pushes the workpiece back into the Storage (6). The process begins anew.

![Diagram](image-url)

**Figure 2.9:** The process flow in the Festo Demonstrator.

In summary, the industrial process is a closed-loop of workpieces (Stock, Storage, Sorting, Processing) that can be entered (Refilling) and exited (Rejects) at one point each, shown in fig. 2.9. The transportation of workpieces through various stations is indicated by arrows. The process is parallelized so that at same time there can be up to 6 workpieces in Stock, 8 workpieces in Storage, 2 workpieces in Sorting, 2 workpieces in Processing and 10 workpieces in Rejects. The Emergency Stop when activated instantaneously disconnects power supply to moving actuators.

### 2.5.2 Industrial Network Communication

The industrial process is controlled through network communication between PLCs, I/O devices, actuators and process-associated sensors, and PLCs with MES and HMI. The process control is divided into 3 production cells, each with its own control system, as shown in fig. 2.10. The direction of arrow indicates Master-to-Slave control in the process.
2.5 System under Consideration

**Figure 2.10**: Different production cells of the Festo Demonstrator.

**Cell 1 “Turntable”**. The PLC-1 controls the *Turntable-Motor* of Storage, and bus coupler BK-1 that relays digital/analog IO signals to the pneumatically operated *Gripper*. The PLC-1, Turntable-Motor, BK-1 and associated sensors are part of Cell 1.

**Cell 2 “Belt”**. The PLC-2 controls the bus coupler BK-2 that relays digital/analog IO signals to upper conveyor *Belt* to move. The PLC-2, BK-2 and corresponding sensors constitute Cell 2.

**Cell 3 “Lift”**. The PLC-3 controls the Lift-Motor of Lift, and bus coupler BK-3 that relays digital/analog IO signals to pneumatic *Pistons* at lower and upper end of the Stock. The PLC-3, Lift-Motor, BK-3 and necessary sensors are part of Cell 3.

The PLC-1 controls the HMI, PLC-2 and PLC-3. It is the global *Master* in the industrial process network.
2 Preliminaries

Figure 2.11: The networking infrastructure of the Festo Demonstrator.

In fig. 2.11, the network infrastructure (physical topology) of the Festo Demonstrator is shown. All the components are connected in STAR topology with the Network Switch at the center. The PLCs communicate to bus couplers and motors through PROFINET protocol, whereas PLCs to HMI communication is through S7Comm protocol. The process information is relayed to MES through OPC UA protocol from OPC UA-compatible PLCs. In case of non OPC UA-compatible PLC-3, an OPC UA gateway collects information from PLC-3 through S7Comm and relays it to MES. RDP protocol is used to connect MES server to a Tablet to visualize the process execution.

2.5.3 Industrial Network Attack Scenarios

An adversary is assumed to have gained access to the Festo Demonstrator’s network infrastructure. In addition, it has the knowledge on the employed industrial components and process parameters being exchanged. Two attack scenarios exist where the adversary targets the industrial process through (i) changing the industrial component’s configuration to make it unavailable for communication (‘Rename Attack’), and (ii) setting the PLC into “FORCE” operational mode to enforce change in the process parameters for an industrial component (‘Force Attack’).
**Rename Attack.** Within PROFINET networks, the components are addressed through their logical names for process data exchange (more details in section 3.3) via the unencrypted PROFINET protocol. An adversary exploits the PROFINET protocol design flaw and changes the logical name of Turntable-Motor to “ufo” via the PN-DCP protocol as shown in fig. 2.12. As a result, the other industrial components are not able to identify the component with the name “Turntable-Motor” and the process stops. Further details on PN-DCP and its role within PROFINET communication will be presented in section 3.3.2.

**Force Attack.** In certain events, an industrial component of the process is faulty and doesn’t communicate the process parameters required for the industrial process to move forward. The process parameters for the faulty component can be “forced” to be sent in the process by the Engineering Tool, such as the TIA-Portal for Siemens PLCs, for the process continuation. An adversary with the knowledge of the Festo Demonstrator’s process, enforces PLC-2 to change the “direction” process parameter of BK-2 and reverses the lower conveyor Belt’s direction, as shown in fig. 2.13.
2 Preliminaries

Figure 2.13: The Force Attack on the Festo Demonstrator.

2.5.4 Network Traffic Capture

For development and evaluation of the analytical methodologies proposed in the presented work, the network traffic from the Festo Demonstrator is captured through its Network Switch. In particular, one of the network interfaces on the Switch is configured to mirror the traffic passing through it and is termed as the “Mirror Port”. The network traffic is captured for two use cases:

1 **Baseline Behaviour.** Normal operation of the process is captured to “learn” the normal behaviour characteristics by the analytical methodologies. No attacks are executed during the capture, and Baseline Dataset row of table 2.3 summarizes the captured data.

2 **Anomaly Detection.** In order to test the performance of analytical models in distinguishing normal traffic from anomalies, the attack scripts are executed during the normal operations. The complete traffic inclusive of attack scripts execution and normal operations is captured for anomaly detection performance evaluation. The information on the captured data is summarized in Evaluation Dataset row of table 2.3.
2.5 System under Consideration

Table 2.3: Summary of datasets captured from the Festo Demonstrator’s communication traffic.

<table>
<thead>
<tr>
<th>Dataset Type</th>
<th>Network Packets Count</th>
<th>Process Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baseline Dataset</td>
<td>60,523,524</td>
<td>2 hours 06 minutes</td>
</tr>
<tr>
<td>Evaluation Dataset</td>
<td>40,518,174</td>
<td>1 hour 24 minutes</td>
</tr>
</tbody>
</table>

In both the use cases, the industrial process begins with ‘referencing’ phase followed by ‘actual process’ phase. In the ‘referencing’ phase, the industrial components are brought to the initial state of the industrial process. In the following ‘actual process’ phase, the process operations are executed. The ‘referencing’ is crucial and unavoidable in the Festo Demonstrator. Therefore, the captured network packets are distinguished too for the two phases.

In addition, prior to ‘referencing’ phase, the Festo Demonstrator undergoes through System Startup, where all the device configurations are transmitted across via different protocols.

The dataset generated from the Festo Demonstrator, normal and anomalous, is utilized for the development and evaluation of the solutions for self-learning of industrial operation behaviour in chapter 3, and industrial process behaviour in chapter 4 and chapter 5.
3 Self-learn PROFINET-based Industrial Communication Networks

Industrial control networks or industrial networks comprises of communication infrastructure between ICS components and network protocols managing the information flows across the automation system. Industrial network operations have strict requirements for real-time data transmission and deterministic communication. It entails further requirement of low jitter from the industrial network protocols to transmit data periodically and maintain strict order for the automated processes [Mes18]. Alarms and diagnostic information must be transmitted aperiodically at occurrence and request, respectively.

Proprietary fieldbus protocols were developed to satisfy these requirements such as PROFIBUS, Modbus, etc. PROFINET is the result of adapting PROFIBUS to real-time technology and standardized in IEC 61158 & IEC 61784. PROFINET Input/Output (PNIO) is the variant developed for distributed Input/Output (I/O) with provider-consumer distribution model for data exchange. It has RT and IRT channels for cyclic process data exchange with average cycle times of $50 - 100\, ms$ and $< 1\, ms$, respectively. RT channel is used for acyclic alarm transmission and UDP/IP channel for acyclic diagnostic data exchange. In addition, PROFINET defines different classes of components characterized by their functionality and participation at different stages of industrial communication - IO Controller, IO Supervisor and IO Device. The transmission of data from IO Controller/Supervisor to IO Device is designated as output data whereas IO Device to IO Controller/Supervisor is input data [V P18].
In this chapter, the challenges encountered in self-learning the industrial operation behaviour of a PROFINET-based system from its monitored traffic and the proposed solutions are outlined. The section 3.1 formulates the research problems followed with the foundational information on PROFINET in section 3.2. In section 3.3, the different networking operations executed through different network protocols in PROFINET systems and their corresponding data frame structures are provided. The proposed framework to enumerate and track the PROFINET operations from the analysis of traffic data is summarized in section 3.4. The section 3.5 presents the framework’s usage for anomaly detection along with the chapter’s review and conclusion.

3.1 Research Problem

Insights into the industrial system’s operation are required for efficient monitoring and timely incident, cyber and physical, response. Interpretation of industrial system operations from its communication network characteristics contributes to being vigilant of cyber threats aimed at industrial process disruption. The networking operations such as neighbourhood detection, connection establishment that an industrial communication network undergoes contains all the required information for network monitoring. The industrial network’s topology, communication relations, assets and protocol data being exchanged during the industrial process operation are the network information to be extracted from the network traffic passively. The challenge being addressed in this chapter is the detection of the different industrial operations from start-up to process data exchange from the network traffic in a systematic way for a self-learning approach.

In addition, the industrial operations executed in an order create the foundation for process data exchanges realizing the underlying intended process. Enumerating these operations through the analysis of multiple protocol communications observed in the traffic and tracking their executions helps to define the industrial system’s operation behaviour. The addition of a device to the network and a device’s attempt to establish communication for process data exchange triggers execution of network operations. Monitoring
the valid operations of devices, communication links or the industrial system would detect the adversarial actions in the context of employed Industrial Ethernet technology’s network protocol communication specifications. In this chapter, the challenge of representing and enumerating a PROFINET system’s operations from monitoring the multiple protocol communication in the network traffic for self-learning an industrial system’s operation behaviour is addressed. The enumerated industrial operations are furthermore tracked to detect deviations for anomaly detection in industrial system.

Interpreting PROFINET-based system operations from network traffic in a systematic way to make the network transparent for downstream analysis, such as modelling underlying ordered periodic and deterministic behaviour of industrial automation systems, is the research problem being addressed in this chapter. It is further formulated as following research questions:

1. How to extract PROFINET-based system operations from network traffic? [Addressed in section 3.3]
2. How to enumerate and track PROFINET-based system operations from network traffic? [Addressed in section 3.4]

3.2 Foundations

TCP (UDP)/IP communication model doesn’t suffice to the industrial communication requirements of deterministic time responses and isochronous communication. Transmission duration of UDP/IP frames inclusive of processing time of a frame through standard communication stacks are found to be non-deterministic [Wil18]. A trimmed down version of communication stack is needed to be defined for real-time PROFINET communication.

For real-time data exchange, emphasis was put on omitting the management & extensive address information transmission, hence, eliminating Session & Presentation layer headers. The real-time frame doesn’t have a Network layer header as it is not passing through any router. Generally the data to be transferred in real-time frame is way less than the standard Ethernet frame’s 1518
bytes, there is no need of segmentation & reassembly of data omitting Transport layer header. Each PROFINET frame is identified by its IEEE assigned Ethertype 0x8892 contained in its VLAN tag for optimal processing by a device. Every PROFINET frame contains Frame ID which defines the associated communication channel of the connection. An UDP/IP protocol based on OSF DCE RPC is used to establish a connection between the controller and device before the real-time data exchange begins.

There are two real-time properties of PROFINET communication: non-synchronized real-time communication (RT) and synchronized real-time communication (IRT). Within PROFINET, process data and alarms are transmitted with RT communication with bus cycle times in the range of milliseconds. Isochronous data transfer with IRT communication are used in applications such as motion control requiring bus cycle times in range of microseconds.

PROFINET utilizes the provider-consumer model of communication for I/O data exchange between controllers and devices, as well as parametrization and diagnosis information exchange between supervisors and devices. PROFINET provides following communication services:

1. Cyclic real-time I/O data exchange between provider and consumer at parametrized increments.
2. Acyclic real-time transmission of acknowledged alarm in the case of system-defined & user-defined events related to controlled process.
3. Acyclic transmission of parameters & diagnostic information for configuring devices and reading out their status information.

PROFINET further defines 3 real-time classes for data exchange: RT_Class_1, RT_Class_3, RT_Class_UDP. RT_Class_1 is used for non-synchronized real-time communication within a subnet, where the minimum transmission cycle is generally 128 ms. The controller defines the time base of the cycle for the transmission of input data of devices. Each device adheres to its time interval for sending its input data. There is no synchronized start of bus cycle for
all the devices. RT_Class_1 frames with VLAN tags are prioritized over UDP/IP frame by a standard industrial switch. RT_Class_3 involves optimized synchronous communication within a subnet where process data is sent in a specific order with maximum precision of 1 microseconds allowed jitter. This is referred as isochronous real-time functionality of PROFINET, where all the participating devices in IRT communication follow the strict order of data transmission. RT_Class_3 frames are transmitted without a VLAN tag through special isochronous capable hardware. RT_Class_UDP is used when real-time frames need to be sent non-synchronized between different subnets. RT_Class_UDP frames contain the destination network address and are transmitted without VLAN tags.

PROFINET defines following classes of components which participate in the industrial communication and drive the industrial process:

- **IO Controller**: It is the component with master functionality that executes the automation program, typically a PLC. It participates in parametrization, cyclic/acyclic data exchange and alarm processing with connected field devices. As the provider, it sends output data to devices and consumes input data from them.

- **IO Supervisor**: An IO Supervisor is used for the commissioning and diagnostic purposes. This is generally a programming device, personal computer or HMI.

- **IO Device**: It is a field device in the vicinity of process with slave functionality that sends process data and critical statuses (alarms & diagnostics) to connected IO Controller(s) via PROFINET. It consumes output data from controller(s) and acts as the provider to send input data to them.

An IO Device comprises of an Ethernet interface for communication and physical/virtual modules to handle the process data traffic. The device model of an IO Device consists of slots, subslots, modules, submodules and channels. The slot and subslot designates the insert slot of a module and submodules in an
IO field device, respectively. The modules provide the structuring and its sub-modules contain the implemented actual inputs and outputs channels. A module contains at least one submodule which always contains the process data with status information. The data within the submodule is addressed using an index. Cyclic IO data in submodule are accessed through slot/subslot combinations, whereas, acyclic read/write services utilize slot, subslot and index.

![Figure 3.1: An example industrial system’s network topology & asset inventory.](image)

A **PROFINET** system contains at least one IO Controller and one or more IO Device. The IO Supervisor is used temporarily for commissioning or troubleshooting purposes, however, it is capable of taking over the control of a device for the supervision of process.¹

All the **PROFINET** components are connected via Switches in an automation system. Within the **PROFINET** communication network, a network asset’s Ethernet interface is defined by its MAC address, IP address and name. When

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¹ Hereafter, the references to device(s) and controller(s) mean IO Device(s) and IO Controller(s).
devices have additional switch ports, each port is identified by its MAC address. Port MAC addresses are used to avoid relearning of Switches’ internal address table whenever their are different paths from same device. All these information constitute an Asset Inventory entry (example in fig. 3.1) of components which is maintained throughout its usage.

There are two variants of network topology observed based on bus structures: 
*star topology*, where multi-port industrial Switches are at the center with each port occupied by a PROFINET device, and 
*line topology*, where devices with integrated Switches are connected in a line. If one of the switch port fails in the line topology, the communication is interrupted, therefore, redundant paths have to be planned beforehand.

### 3.3 Network Operation Enumerations for **PROFINET**

Configuration and commissioning of **PROFINET**-based automation systems must follow certain mode of operations in a strict order. It begins with the System Engineering operation where an automation project is configured in an engineering tool. General System Description (GSD), an XML file provided by every device manufacturer, contains configuration information for parametrizing the devices for real systems. In addition, each device is assigned a logical name to address it within the **PROFINET** communication. Within the System Engineering mode, an IP address is assigned to each device for communication. Transmission intervals are defined for cyclic data exchange between controller and devices. After system engineering is completed, the configuration information is downloaded to the controller. As soon as the automation system is powered on (or reset), Neighbourhood Detection, Address Resolution and System Startup are the operations followed in the same order, as shown in fig. 3.2. With Address Resolution, the controller uses the system configuration information to assign the IP addresses to the devices identified through their pre-assigned logical names. System Startup operation mode is
initiated by the controller to establish connection with devices and configure their I/O parameters. When the I/O parametrization ends successfully, the controller and devices step into Data Exchange mode to transmit process data, alarms and diagnostic information throughout the network.

![Figure 3.2: Networking operations of an industrial system.](image)

Every mode of operation, from configuration to commissioning the PROFINET-based automation system, is accomplished through a complementary network operation involving specific network protocols. *Link Layer Discovery Protocol (LLDP)* is associated with Asset Discovery & Neighbourhood Detection networking operations to accomplish the Neighbourhood Detection PROFINET operation. The Address Resolution networking operation is performed by *PN-DCP* and *Address Resolution Protocol (ARP)* to execute Address Resolution PROFINET operations. The System Startup PROFINET mode involves *PROFINET Context Manager (PN-CM)* protocol reflecting Connection Establishment networking operation. *PNIO* protocol is associated with Data Exchange networking mode to achieve the Data Exchange PROFINET operations.

Enumeration of PROFINET operation modes is performed by passively monitoring/analysing the network traffic and identifying the associated network operation stage-by-stage. System Engineering mode is performed offline, hence, it can’t be enumerated through analysing the network traffic.

In the following subsections, we will dive into each of the networking operations. For every network operation, the role it plays within PROFINET-based automation system communication and the network protocol utilized to achieve the goal will be outlined. The information extracted through dissecting protocol traffic and its usage in filling the asset inventory and network topology model are also presented.
3.3 Network Operation Enumerations for PROFINET

3.3.1 Asset Discovery & Neighbourhood Detection

After the automation system is powered on, the field device’s MAC interface and its Physical Device Management (PDev) gets activated to start transmitting the parameters. PDev contains hardware-level information such as interface name, switch port data, interface and Port MAC addresses and reten-tively stores IP address and logical name assigned to the device. Port information is used by devices to determine their neighbours on port-by-port ba-sis. Neighbourhood Detection is accomplished through LLDP services as part of PROFINET’s overall concept “Device Replacement Without Engineering Tool”. LLDP-capable devices communicate with their connected neighbours to cyclically exchange addressing information and consequently determine their physical location. A controller can use PN-DCP or Simple Network Management Protocol (SNMP) to query the LLDP information from devices and re-produce the system topology. When a field device is replaced with new MAC address, the system topology information stored by the controller is used to commission the new device automatically using it’s assigned logical name.

An example of LLDP frame structure is shown in fig. 3.3. LLDP frames are identified through their IEEE-assigned Ethertype 0x88CC with fixed multicast MAC address 01-80-C2-00-0E. Source MAC address is Port MAC address of sending device’s switch port. LLDP Data Unit (LLDPDU) contains chain of information blocks called Type Length Value (TLV) fields: Chasis ID, Port ID, Organization Identifier (OID), Time To Live (TTL) and End of LLDPDU. Chasis ID corresponds to device’s name. Port ID value has the form PORT-001, if one switch port is present, else PORT-001-RSTUV for multiport switches, where RSTUV represents the slot number. OID has value 24686 if PROFINET device else 0 when no value is provided by the manufacturer. TTL specifies the update time to ensure consistent data management and LLDP information validation.

<table>
<thead>
<tr>
<th>Ethertype</th>
<th>Link Layer Data Protocol Data Unit (LLDPDU)</th>
<th>Padding Optional</th>
<th>FCS</th>
</tr>
</thead>
<tbody>
<tr>
<td>0x88CC</td>
<td>Chasis ID, Port ID, TTL, OID, ...</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 3.3: The structure of a LLDP frame.
LLDP frames are dissected to identify device names, number of switch ports and their MAC addresses for the Automated Asset Inventory, developed for the analysis in the reported work. Fig. 3.4 shows an example of attributes added for the device *Lift-Motor* of the *Festo Demonstrator* (refer section 2.5).

**Figure 3.4:** The demonstration of *Lift-Motor* device’s Asset Inventory filled with information from LLDP frame (*Wireshark* snippet).

### 3.3.2 Address Resolution

Before the *PROFINET*-based automation system starts up and field devices start communicating, an IP address needs to be assigned to all devices by the controller. An IO Device is identified through its ‘*NameOfStation*’ information stored in its PDev and an IP address defined during System Engineering mode is assigned to it. Address Resolution networking operation for every device takes place step-by-step as follows:

1. Controller starts with name resolution and checks for device with configured name through ‘*DCP Identify*’ service of *PN-DCP*.
2. Address Resolution begins with checking if the IP address already exists to avoid assigning same IP address twice through *ARP*.
3. At the end of networking operation, the IP address is assigned to configured device through ‘*DCP Set*’ service of *PN-DCP*.

The schematic communication order for Address Resolution between *PLC-3* and *Lift-Motor* is shown in fig. 3.5.
3.3 Network Operation Enumerations for PROFINET

Figure 3.5: The Address Resolution handshake between PLC-3 and Lift-Motor.

Frame structures of DCP Identify, ARP and DCP Set are outlined below with a brief description of relevant fields.

**DCP Identify** is the real-time service of PN-DCP with Ethertype 0x8892 and fixed PI multicast MAC address 01-0E-CF-00-00-00 for request frames. DCP Identify request and response frames are identified through their service identifiers in DCP Header with values 5.0 and 5.1, respectively (fig. 3.6). DCP Data field contains name of the device which is being checked for availability. DCP Response field is contained only in response frame instead of DCP Data to confirm the availability of device with searched name and parameters.

**ARP** is the standard IT service for IP resolution with Ethertype 0x0806. The controller sends an ARP request with broadcast destination MAC address FF-FF-FF-FF-FF-FF to all devices checking for IP address availability. At the startup,
since none of the devices are assigned any IP address, there won’t be any ARP response frames. ARP request and response frames are identified by their operation code in OPER field with values 1 and 2, respectively. SHA, SPA, THA and TPA fields correspond to hardware (MAC) address and protocol (IP) address of sender and target, respectively (fig. 3.7). In request frame, THA is broadcast address, TPA is the IP address query, SHA and SPA are MAC and IP address of the controller.

<table>
<thead>
<tr>
<th>Ethertype</th>
<th>OPER</th>
<th>SHA</th>
<th>SPA</th>
<th>THA</th>
<th>TPA</th>
<th>FCS</th>
</tr>
</thead>
<tbody>
<tr>
<td>0x0806</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Figure 3.7:** The structure of an ARP frame.

DCP Set is the real-time service of PN-DCP with Ethertype 0x8892. DCP Set request and response frames are identified through their service identifiers in DCP Header with values 4.0 and 4.1, respectively (fig. 3.8). With DCP Set request frame, the controller writes IP parameters contained in DCP Data field to a device.

<table>
<thead>
<tr>
<th>Ethertype</th>
<th>Frame ID</th>
<th>DCP Header</th>
<th>DCP Data</th>
<th>FCS</th>
</tr>
</thead>
<tbody>
<tr>
<td>0x8892</td>
<td>Service Identifier = 4.0/4.1</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Figure 3.8:** The structure of a DCP Set frame.

The information dissected from an ARP request packet is used to add the IP address to controller assets. Information dissected from DCP Set is used to add IP address information to configured devices, example shown in fig. 3.9.
3.3 Network Operation Enumerations for PROFINET

3.3.3 Connection Establishment

System Startup operation begins with establishment of communication relationships between the controller and devices via PN-CM communication exchanges. Through these established communication the controller transmits all the parameters for process data exchange to the internal module of devices. The process model and associated parameters for devices participating in the process are engineered & defined during System Engineering operation.

The ‘connection’ between an IO Controller and an IO Device is established in an ‘Application Relationship (AR)’ uniquely identified by an ARUUID. An ARUUID is generated by the engineering tool for specific system configuration & device. Within this AR, different ‘Communication Relationship (CR)’ are established for different data exchanges. A device can be connected to multiple controllers through different ARs. An application can access data only through CRs established in an AR.

IOC-AR, IOS-AR and Implicit AR are different ARs defined by PROFINET. The IOC-AR (Controller AR) is between controller and device for cyclic data exchange of input & output data, read/write of acyclic data and alarms transmission. The IOS-AR (Supervisor AR) is between supervisor and device with properties same as IOC-AR. Implicit AR is between a controller/supervisor and device for the sole purpose of acyclic reading of data from device.
Different ‘Communication Relationship (CR)’ are defined by PROFINET for different data requirements. IO-Data CR (IOCR) is the IO data communication relationship established for cyclic process data exchange in real-time. The controller transmits in IOCR various parameters for cyclic data exchange: transmission frequency, data length, specification of input/output data, sequence of transmitting data, etc. The controller can set up multiple IOCR with a device for different data objects with different transmission frequencies. The transmission frequency defines the fixed interval cycle for data exchange between controller and device in both directions (input & output). Alarm CR is established along with an IOCR for acyclic bidirectional transmission of process and diagnostic alarms via the real-time channel. Record Data CR is established for acyclic data exchange to read diagnostic, log and device data. It is explicitly used for writing the configuration and AR data.

A ‘connection’ between a controller and a device is defined the least by 1 AR, 2 IOCR (input & output), 1 Alarm CR and 1 Record Data CR. PROFINET offers PN-CM protocol to handle the Connection Establishment network operation. The PN-CM network operation uses UDP/IP channel to transmit following frames in the strict order for establishing ‘connection’ between controller and device:

- Connect frames establish AR and CRs channels.
- Write frames parametrize the device submodules.
- DControl frames mark the end of parametrization from the controller.
- CControl frames mark the validation check of parameters, data structure build up and application readiness from the device.

The first successful exchange of I/O data after CControl frames mark the end of PROFINET’s System Startup operation mode. The schematic communication order for Communication Establishment between PLC-3 and Lift-Motor is shown in fig. 3.10.
3.3 Network Operation Enumerations for PROFINET

Frame structures of *Connect*, *Write*, *DControl* and *CControl* are outlined below with a brief description of relevant fields. All *PN-CM* frames are transmitted with Ethertype=0x0800.

![Figure 3.10: The Connection Establishment handshake between PLC-3 and Lift-Motor.](image)

A *Connect request* frame is sent from controller to device containing parametrization information for transmission frequency, length and order of process data, input & output data specification related to *submodules* and *subslots* of device. Any error in the parametrization information (such as absence of *submodule*) is notified by the device in a *Connect response* frame. *RPC* contains the data transmission format value either *Big Endian* or *Little Endian*. *AR Block* contains *ARUUID* and relevant information to establish AR between controller and device. *CR Input* and *CR Output* are the blocks with instructions for input and output data transmission including transmission frequency (refer fig. 3.11). *ExpSubm* is only present in *request* frames containing identification.

![Figure 3.11: The structure of a PN-CM Connect frame.](image)

<table>
<thead>
<tr>
<th>Ethertype</th>
<th>IP UDP</th>
<th>RPC</th>
<th>AR Block</th>
<th>CR Input</th>
<th>CR Output</th>
<th>CR Alarm</th>
<th>ExpSubm</th>
<th>Module Diff</th>
<th>FCS</th>
</tr>
</thead>
<tbody>
<tr>
<td>0x0800</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
of device’s modules and submodules to be parametrized for process data exchange. ModuleDiff is present only in response frames in the case of error in setting up device’s modules and submodules.

Figure 3.12: The structure of a PN-CM Write frame.

The Write frame has a Write Block field containing information for addressing the data objects of submodules and its length (refer fig. 3.12). The Write Data field is only present in a Write request frame from controller to device and contains the parametrization data for the addressed data object.

Figure 3.13: The structure of a PN-CM DControl frame.

DControl request frame is sent from controller to device notifying the end of parametrization and the device acknowledges it in the response frames (refer fig. 3.13).

Figure 3.14: The structure of a PN-CM CControl frame.

A CControl request frame is sent from device to controller indicating its application readiness (refer fig. 3.14). It might contain ModuleDiff to notify error in writing data/parameters to identified submodules. If no ModuleDiff is found
by the controller in the \textit{CControl request} frame, it acknowledges device’s application readiness in \textit{response} frame. With this frame, the AR is established and all the frames required for startup are transmitted.

The GSD of a device contains modules and submodules information reflecting the position of process data within the payloads. Since in a self-learning analysis from network traffic the GSD isn’t accessible, the aforementioned information is extracted through reading and interpreting \textit{Connect} frames. \textit{PN-CM} frames are dissected to extract the input and output data specifications for device’s submodules. It contains the data format type (endianess), order of data, length of data and the position of data within the payload bytes. An example of payload bytes of input data frames without network header information is shown in fig. 3.15.

![Figure 3.15: The demonstration of extracting Input Data parameters between PLC-3 and Lift-Motor from Connect frame (Wireshark snippet).](image)

These specifications are used in Data Exchange network operation’s \textit{PNIO} frames to extract process bytes. The ‘connection’ between controller and device following a Connection Establishment network operation guides building the logical network topology of the system. These separated ISO layer
connection state information between network assets is maintained throughout the automation system’s runtime and deviations are reported, an example shown in fig. 3.16.

![Logical network topology between PLC-3 and Lift-Motor.](image)

**Figure 3.16:** The logical network topology between PLC-3 and Lift-Motor.

### 3.3.4 Data Exchange

Once the System Startup operation establishes AR and data specific CRs between devices and controller, the connection-oriented communication channel is set for exchange of cyclic process data, acyclic diagnostic data and alarms. Cyclic process data are transmitted in real-time in IOCR channel whereas Record Data CR transmitted acyclic data via UDP/IP. PNIO protocol defines the format and context for data exchange.

Cyclic PNIO frames are sent unacknowledged between controller and devices. The validity of transmitted data is exchanged through status information in field IOPS (Input Output Provider Status) and IOCS (Input Output Consumer Status) by the provider and consumer, respectively. After CControl frames are acknowledged by the controller, the first valid exchange of I/O data with IOPS=GOOD ends Connection Establishment operation. Data Exchange operation begins with cyclical exchange of process data at configured/parametrized fixed intervals.

![Structure of a PNIO frame.](image)

**Figure 3.17:** The structure of a PNIO frame.
PNIO cyclic data frame is transmitted in real-time with Ethertype=0x8892 and its structure outlined in fig. 3.17. Frame ID distinguishes between cyclic and acyclic real-time frame. The process data bytes from Data field are extracted using information from Connect frame dissection, as shown in fig. 3.18.

3.4 PROFINET Operations Enumeration and Tracking

Through monitoring an industrial system’s communication network, its characteristics are observed to build normal operations behaviour baseline. Deviations from the baseline behaviour could be triggered by physical or cyber threats. A systematic framework is needed to enumerate operations extracted from network traffic and track them to report deviations.

PROFINET-based automation systems follow strict order of operations. The operation mode and corresponding network operations with associated network protocols have been outlined in section 3.3. All of those network operation’s dissected information are combined to systematically iterate over
the PROFINET operation modes as and when there occurrences are observed through network analysis. PROFINET devices transit through PROFINET operations to establish connections between them for cyclic and acyclic data exchange. These transitions also govern transitions in PROFINET connections, which constitutes the logical topology and industrial process behaviour of the PROFINET system.

Finite State Machines (FSM) [Kle56] are widely used for protocol specification (e.g. TCP/IP [Ste93]) [Hol93], where the valid transitions and states of message exchanges are defined [Reu02]. For the requirements of capturing the transitions between industrial operations triggered by the communication events, the FSMs are modelled to enumerate the PROFINET operations of the device, connection and system. PROFINET standard, the informative handbook on PROFINET [Pop14] and empirical information collected from analysing real-world PROFINET-based system communications are interpreted to model the operations in FSMs.

In the next subsections, each FSM is described with the overview of states and events triggering the transitions outlined in its state diagram. The transitions which are modelled based on empirical information are distinguished by dashed edges and details are presented. The FSM diagrams are accompanied with tabular details on source and target state, triggering event, protocol frame used for event detection and underlying PROFINET network operation of transition. Each row of the table represents a transition of FSM.

3.4.1 FSM PROFINET Device

States and transitions. FSM Device enters with Active state as soon as the system is powered on, shown in fig. 3.19. It transits either to Neighbourhood Detection or Name Resolution state depending on the event triggered. FSM follows through the transitions as and when the triggering event is detected in network traffic. The protocol frame triggering the events for PROFINET operation transitions of a device are summarized in table 3.1.
Figure 3.19: PROFINET Device State Machine.
LLDP frames are periodically transmitted by PROFINET device as per their TTL value for consistent LLDP information validation (refer section 3.3.1). Hence, Neighbourhood Detection state can be arrived from any other state whenever detect_neighbours event is triggered by LLDP frame. Consequently, all the states are reachable with corresponding triggering events from Neighbourhood Detection state.

Table 3.1: Summary of FSM Device transitions with triggering event, event detection protocol and PROFINET operation.

<table>
<thead>
<tr>
<th>Source</th>
<th>Target</th>
<th>Trigger Event</th>
<th>Protocol Frame</th>
<th>PROFINET Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Active</strong></td>
<td>Neighbourhood Detection</td>
<td>detect_neighbours</td>
<td>LLDP</td>
<td>Asset Discovery</td>
</tr>
<tr>
<td>Name Resolution</td>
<td>Name Resolution</td>
<td>identify_device</td>
<td>DCP Identify request</td>
<td></td>
</tr>
<tr>
<td>Neighbourhood Detection</td>
<td>Name Resolution</td>
<td>device_identified</td>
<td>DCP Identify response</td>
<td></td>
</tr>
<tr>
<td>Neighbourhood Detection Name Resolution</td>
<td>IP Address Assignment</td>
<td>assign_ip</td>
<td>DCP Set request</td>
<td></td>
</tr>
<tr>
<td>Neighbourhood Detection</td>
<td>IP Address Assignment</td>
<td>ip_assigned</td>
<td>DCP Set response</td>
<td></td>
</tr>
<tr>
<td>IP Duplication Check IP Address Assigned</td>
<td>IP Duplication Check</td>
<td>check_ip_duplication</td>
<td>ARP (Gratuitous ARP)</td>
<td></td>
</tr>
<tr>
<td>Neighbourhood Detection</td>
<td>New Connection Initiated</td>
<td>create_connection</td>
<td>Connect request</td>
<td></td>
</tr>
<tr>
<td>Name Resolved</td>
<td>Parametrization</td>
<td>initiate_parametrization</td>
<td>Write</td>
<td></td>
</tr>
<tr>
<td>Neighbourhood Detection</td>
<td>Parametrization</td>
<td>write_parameters</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Neighbourhood Detection</td>
<td>End Of Parametrization</td>
<td>end_parametrization</td>
<td>DControl request</td>
<td></td>
</tr>
<tr>
<td>New Connection Initiated</td>
<td>Application Ready</td>
<td>parmeterization_success</td>
<td>CControl response</td>
<td></td>
</tr>
<tr>
<td>Neighbourhood Detection</td>
<td>Connection Established</td>
<td>device_configured</td>
<td>PNIO</td>
<td></td>
</tr>
<tr>
<td>Parametrization</td>
<td>Data Exchange</td>
<td>initiate_process</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Neighbourhood Detection</td>
<td>Data Exchange</td>
<td>process_data_sent</td>
<td>PNIO</td>
<td></td>
</tr>
<tr>
<td>Acyclic Reading Data</td>
<td>Acyclic Reading Data</td>
<td>acyclic_data_read</td>
<td>Read</td>
<td></td>
</tr>
<tr>
<td>Acyclic Parametrization</td>
<td>Acyclic Parametrization</td>
<td>acyclic_data_write</td>
<td>Write</td>
<td></td>
</tr>
</tbody>
</table>
3.4 PROFINET Operations Enumeration and Tracking

Through network traffic analysis of PROFINET-based systems with Siemens PLC, transitions - IP Address Assignment to IP Address Assigned and IP Address Assigned to IP Duplication Check - have been modelled. Deviating from transitions mentioned in the literature, the PROFINET devices checked for IP duplication with Gratuitous ARP after the IP address has been assigned to them. These transitions are verified on different PROFINET-based systems available at IT-SECURITY LAB, FRAUNHOFER IOSB.

**Relationship between states and PROFINET operations.** The transitions between states reflecting progress of PROFINET operations of a device are outlined in table 3.1. Neighbourhood Detection state constitutes Asset Discovery & Neighbourhood Detection PROFINET operation. States Name Resolution, Name Resolved, IP Address Assignment, IP Address Assigned and IP Duplication Check constitute Address Resolution PROFINET operation. PROFINET’s Connection Establishment operation consists of states New Connection Initiated, Parametrization, End Of Parametrization, Application Ready and Connection Established. States Data Exchange, Acyclic Parametrization and Acyclic Reading Data reflect Data Exchange PROFINET operation.

### 3.4.2 FSM PROFINET Connection

![PROFINET Connection State Machine](image)

**Figure 3.20:** PROFINET Connection State Machine.
**States and transitions.** A **PROFINET** connection is established between **PROFINET** devices through **PROFINET**’s PN-CM protocol handshake (refer section 3.3.3). The cyclic and acyclic data exchange takes place through this connection. Hence, each connection is identified through MAC addresses of participating **PROFINET** devices. FSM Connection enters with *Connection Creation* state as soon as *Connect request* frame is sent by the controller, shown in fig. 3.20. FSM follows through the transitions as and when the triggering event is detected in network traffic. The protocol frame triggering the events for **PROFINET** operation transitions of a connection are summarized in table 3.2. In particular, events *output_process_data_sent* and *input_process_data_sent* are triggered by transmission of PNIO frames from controller to device and vice versa, respectively (refer section 3.3.4).

**Table 3.2**: Summary of FSM Connection transitions with triggering event, event detection protocol and **PROFINET** operation.

<table>
<thead>
<tr>
<th>Source</th>
<th>Target</th>
<th>Trigger Event</th>
<th>Protocol Frame</th>
<th><strong>PROFINET</strong> Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Connection Creation</td>
<td>Connection Configuration</td>
<td><em>initiate_parametrization</em></td>
<td>Write</td>
<td>Connection Establishment</td>
</tr>
<tr>
<td>Connection Configuration</td>
<td>Connection Established</td>
<td><em>device_configured</em></td>
<td>PNIO</td>
<td></td>
</tr>
<tr>
<td>Connection Established</td>
<td>Input Data Exchange</td>
<td><em>initiate_process</em></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Input Data Exchange</td>
<td>Output Data Exchange</td>
<td><em>output_process_data_sent</em></td>
<td>PNIO</td>
<td></td>
</tr>
<tr>
<td>Acyclic Parametrization</td>
<td>Output Data Exchange</td>
<td><em>output_process_data_sent</em></td>
<td>PNIO</td>
<td></td>
</tr>
<tr>
<td>Input Data Exchange</td>
<td>Acyclic Parametrization</td>
<td><em>input_process_data_sent</em></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Input Data Exchange</td>
<td>Acyclic Reading Data</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Output Data Exchange</td>
<td>Acyclic Parametrization</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Output Data Exchange</td>
<td>Acyclic Reading Data</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Output Data Exchange</td>
<td>Acyclic Reading Data</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Relationship between states and **PROFINET** operations.** The transitions between states reflecting progress of **PROFINET** operations of a connection are outlined in table 3.2. States *Connection Creation*, *Connection Configuration* and *Connection Established* constitute Connection Establishment **PROFINET** operation. **PROFINET**’s Data Exchange operation are reflected in states *Input Data Exchange*, *Output Data Exchange*, *Acyclic Parametrization* and *Acyclic Reading Data*. 
3.4.3 FSM PROFINET System

**States and transitions.** FSM System initializes with *Inactive* state and transits into *Powered On* as soon as PROFINET traffic triggers event *pn_traffic_detected*, show in fig. 3.21. FSM follows through the transitions as and when the triggering event is detected in network traffic. The protocol frame triggering the events for PROFINET operation transitions of a system are summarized in table 3.3. Event *all_connections_established* is triggered when all the FSM PROFINET Connection instances have arrived in state *Connection Established*.

![PROFINET System State Machine](image)

**Figure 3.21:** PROFINET System State Machine.

**Table 3.3:** Summary of FSM System transitions with triggering event, event detection protocol and PROFINET operation.

<table>
<thead>
<tr>
<th>Source</th>
<th>Target</th>
<th>Trigger Event</th>
<th>Protocol Frame</th>
<th>PROFINET Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inactive</td>
<td>Powered On</td>
<td><em>pn_traffic_detected</em></td>
<td>LLDP</td>
<td>Asset Discovery</td>
</tr>
<tr>
<td></td>
<td>System Startup</td>
<td><em>new_device_instantiated</em></td>
<td>DCP Identify request</td>
<td>Address Resolution</td>
</tr>
<tr>
<td>System Startup</td>
<td>System Startup</td>
<td><em>new_device_instantiated</em></td>
<td>Connect request</td>
<td>Connection Establishment</td>
</tr>
<tr>
<td>System Startup</td>
<td>Data Exchange</td>
<td><em>all_connections_established</em></td>
<td>PNIO</td>
<td></td>
</tr>
<tr>
<td>Data Exchange</td>
<td>Data Exchange</td>
<td><em>process_data_detected</em></td>
<td>PNIO</td>
<td>Data Exchange</td>
</tr>
<tr>
<td>Data Exchange</td>
<td>Data Exchange</td>
<td><em>acyclic_data_detected</em></td>
<td>Write/Read</td>
<td></td>
</tr>
</tbody>
</table>
Relationship between states and PROFINET operations. The transitions between states reflecting the progress of PROFINET operations of a system are outlined in table 3.3. State Powered On reflects either PROFINET operation Asset Discovery & Neighbourhood Detection or Address Resolution if the event pn_traffic_detected is triggered by LLDP or DCP Identify request frames, respectively. State Asset Configuration & System Startup (referred as System Startup in table 3.3) reflects Connection Establishment PROFINET operation. PROFINET’s Data Exchange operation of cyclic and acyclic data transmission is reflected in state Data Exchange.

3.4.4 POET: A Framework for PROFINET Operations Enumeration and Tracking

PROFINET system, connection and device FSMs are realized in a python-based framework, termed as PROFINET Operations Enumeration and Tracking (POET), for enumeration and tracking PROFINET-based industrial network communication. It is implemented with pytransitions [Pyt] and logs transitions in FSM instances of PROFINET System, Connection and Device continuously. Each FSM PROFINET System instance is identified by a name given while initialization, whereas the device name extracted from network traffic (DCP Identify request/LLDP frame) is used for identifying FSM PROFINET Device instance. FSM PROFINET Connection instance is identified by the connection identifier created from concatenating MAC addresses of devices.

POET clearly satisfies the BSI’s “Category A - general requirements” outlined in section 1.1.1, for an anomaly detection system to identify communicating devices, protocols and communication links (modeled as PROFINET Connection) in the industrial network.
3.5 Discussion and Summary

3.5.1 Anomaly Detection with POET

Industrial networks are vulnerable to different threat behaviours, each utilizing different techniques to exploit industrial network characteristics. MITRE ATT&CK for ICS [Str18] is a knowledge base of such industrial system targeted threat behaviours, collected through cyber threat intelligence reports of known cyber incidents, refer section 2.2. Some threat behaviours (such as Modify Parameter, Denial of Service) are targeted at the industrial network operation to disrupt the underlying industrial process.

Pfrang et al. [Pfr17] outlined threat scenarios targeted at real-world PROFINET-based systems with two different techniques to take over control of a PROFINET device. Within PROFINET networks, the devices are identified through the assigned logical name (refer section 3.3) for process data exchange.

The first attack of [Pfr17] demonstrated how an attacker changes the name of a device utilizing PN-DCP protocol and disconnecting it with other devices. A similar attack was performed on the Festo Demonstrator and POET was employed to monitor network traffic. The attack triggered events which aren’t allowed for FSM Device instance of ‘festo-motor-scheibe’ and were reported in POET’s logger, as shown in fig. 3.25. The blue edges are the valid PROFINET operation transitions triggered by the appropriate protocol events (a, b, ... f) as shown in fig. 3.22 - fig. 3.24. As per the PN-DCP protocol specification, the packets (x) are valid, however, they violate PROFINET device’s valid operation transition represented as red edges, and thus detected.
Figure 3.22: The network events, (a) device_identified, (b) check_ip_duplication and (c) create_connection, triggered by the network packets sent in the traffic of the Festo Demonstrator with the POET.

Figure 3.23: The network events, (d) device_configured and (e) initiate_process, triggered by the network packets sent in the traffic of the Festo Demonstrator with the POET.
3.5 Discussion and Summary

Figure 3.24: The network events, (f) `process_data_sent` and (x) `identify_device`, triggered by the network packets sent in the traffic of the *Festo Demonstrator* with the POET.

Figure 3.25: The detection of Rename Attack on the *Festo Demonstrator* with the POET. The network event “(x) *identify_device*” triggered an invalid transition to ‘Name Resolution’ operation.
[Pfr17] outlined the second attack which is essentially disrupting PROFINET network operations by establishing new connection with device. This action initiates Connection Establishment PROFINET operation which isn’t valid transition state for FSM Device instance. Employing POET in such scenarios would also detect this attack and enhance visibility to unwarranted events in PROFINET networks with explanation.

POET’s capability to detect the two attacks outlined in [Pfr17] satisfies the BSI’s “Category B - unusual or exceptional activities in an ICS network” requirements outlined in section 1.1.1. It identifies the change in protocol communication between industrial components and detects new devices in the network through FSM Device and Connection models. Additionally, any other attacks that would violate the validity of an industrial operation through protocols other than PN-DCP and PN-CM would be detected by POET.

### 3.5.2 Review

Protocol-analysis based IDS have been proposed for industrial protocols such as DNP3, Modbus/TCP, GOOSE, etc. [Hu18], where protocol specifications are utilized to build system profile and the deviations are reported. The proposed FSM-based framework, POET, can be categorized along with them as Protocol-analysis based IDS for PROFINET.

POET is the first-of-its-kind Protocol-analysis based IDS for PROFINET to incorporate empirical behaviour of PROFINET system collected from real-world systems. The current version of POET uses empirical information collected from PROFINET systems incorporating Siemens PLC, it could vary with other PLC environments (eg. CODESYS [17]), devices and can be adapted. The extraction of network events triggering the transitions of industrial operations would be adapted to the new protocol communication stack.

POET offers insights into the operations of PROFINET-based systems at ascending granularity of system, connection between devices and device. This granularity helps to specify events proficiently to be used in downstream analysis for anomaly detection. For example, [Pfr17] outlined enhanced Snort for
PROFINET which was used to detect the two attacks mentioned in their work. It can be integrated with POET to trigger alarms when unwarranted transitions occur.

At the end, this chapter demonstrates a successful workflow to interpret an industrial protocol specification and the empirical information collected from its real-world industrial system usage to design a Protocol-analysis based IDS. A similar workflow could be utilized for another industrial protocol such as EtherNet/IP utilizing the outlined FSM models at different granularities of system, connection and device. The FSM models would have to be adapted for states and triggering events.

3.5.3 Conclusion

In this chapter, the PROFINET network traffic is mapped to different PROFINET operations for interpreting the underlying status of industrial communication. In section 3.3 the solution to research problem 1 is outlined, where different protocols associated with PROFINET operations are mapped to PROFINET network operations. For every network operation, the role it plays within PROFINET-based automation system communication and the network protocol utilized to achieve the goal has been presented. Thus satisfying the BSI’s “Category A - general requirements” for network transparency as outlined in section 1.1.1.

In addition, the protocol associated communication behaviour and their detection through protocol frame analysis has been outlined. As the solution to research problem 2, section 3.4 modelled operations of PROFINET system, connection and device as Finite State Machines (FSM) to systematically enumerate and track PROFINET operations. PROFINET Device, Connection and System FSMs are realized in a python-based framework named PROFINET Operations Enumeration and Tracking (POET). Its successful usage as Protocol-based IDS in detecting cyber attack on real-world PROFINET demonstrator has been presented in section 3.5.1. This demonstrates POET as an anomaly detection solution that satisfies the BSI’s “Category B - unusual or exceptional activities in an ICS network” requirements as outlined in section 1.1.1.
In conclusion, the challenge of self-learning PROFINET-based industrial communication networks is solved through interpretation of network traffic to PROFINET operations. The workflow developed in this chapter to interpret an industrial protocol’s specification with the empirical information from its real-world usage to develop an anomaly detection system can be replicated further.

Data Exchange dominates the PROFINET operations where the actual industrial process is realized. In the next chapter, the research problems associated with analysing the PNIO frames for anomaly detection of industrial process behaviour through Byte Profiling is being addressed.
4 String-based Self-learning Process Behaviour from Network Traffic

An industrial process at its core is the interplay of instruction exchanges between actuators/sensors and controllers of an industrial control network. It could be either of 3 types, characterized by the stationarity of process data: discrete, continuous, or batch [Wil18]. Discrete processes are non-stationary as the process data vary at fixed time intervals and in a fixed order following a time schedule. Automotive, manufacturing and textile industry are its application domains. In continuous processes, the process data output remains temporally constant, and hence is stationary. Petrochemical industry and refineries are some of its application domains. Within batch processes, the goods are processed continuously at fixed time schedules. Breweries, pharmaceutical and food industry are driven in a batch process.

Industrial processes have stringent deterministic requirements to transmit information in real-time with low jitters. Additionally, the process parameters have to be transmitted periodically in a fixed order while maintaining temporal consistency. In order to fulfil high determinism requirements, industrial communication protocols implemented reduced OSI/ISO stack architectures to avoid transmission delays of information processing between layers.

Since 2000, Advanced Persistent Threats (APT) modified the instruction exchanges within industrial processes, utilizing industrial protocols, to cause structural damage to components (Stuxnet) or HSE hazards (Industroyer/ CrashOverride, Triton) [Mak21]. Continuous monitoring and analysis of industrial process could detect the initiation of such attacks and reduce dwell time to accelerate mitigation. The analysis requires understanding the process behaviour of an industrial system to distinguish an anomaly.
from normality. These anomalies represent malfunctioning of components due to modification of process parameters or change in overall industrial process logic as effects of the cyber threat. In a self-learning setup, where the information on process parameters is not at one’s disposal, the process behaviour is interpreted through analysis of industrial network traffic. With chapter 3 as foundational knowledge on PROFINET operations, in this chapter, the discrete process behaviour of PROFINET-based industrial system is modeled from its network traffic.

In order to understand the underlying industrial process from PROFINET network traffic, a closer look at constituents and characteristics of industrial process is required. An industrial process encompasses multiple sub-processes that are executed in periodic order at deterministic intervals as programmed during System Engineering PROFINET operation (refer section 3.3). Each sub-process is represented by the connection between a pair of controller and device, established through PN-CM protocol (refer section 3.3.3). Within this sub-process, the process data consisting of process parameters are exchanged periodically in strict intervals. The periodic and deterministic requirements of industrial process defines its spatio-temporal characteristics. In particular, the periodicity in process data exchange represents the spatial characteristic, and deterministic intervals the temporal characteristic of an industrial process and its constituent sub-processes. In addition, the production cycle of industrial process is defined by the deterministic and periodic execution of process parameters of constituent sub-processes.

This chapter addresses the challenge of representing the spatio-temporal characteristics of an industrial process as String and self-learning the process behaviour for anomaly detection. In section 4.1, the research problems concerning representation and learning are formulated. The solutions are proposed in section 4.2 - section 4.5. In section 4.6, the usage of the proposed framework for production cycle and anomaly detection tasks on the Festo Demonstrator are presented. The section ends with chapter’s review and conclusion.
4.1 Research Problem

An adversary targets the industrial process through exploiting its spatial and temporal characteristics. With the knowledge of process parameters and employed industrial components, the adversary could either change the component configurations or process parameters. The manipulation of process parameters could be triggered to:

i. set the component in an operation state that violates the execution order of the process’ constituent sub-process parameters (spatial characteristic exploitation).

ii. delay the communication between process parameter exchanges to have cascading effect on the process (temporal characteristic exploitation).

Protocol analysis-based Intrusion Detection Systems (IDS), such as POET (refer section 3.4.4), and traffic mining-based IDS does not have insights into the process data being exchanged in an industrial control network. Hence, process analysis-based IDS with insights into industrial process characteristics are employed for detecting the adversary’s actions [Hu18]. In general, process variables are known to the process analysis-based IDS for process behaviour analysis [Had14, Cas15, Ant19, Por21]. As already pointed out previously, in a self-learning setup, the explicit knowledge on process variable is not available, the process behaviour needs to be interpreted through analysing the industrial network traffic.

In chapter 3, the communication handshake between a Controller and Device to establish a connection as channel for cyclic and acyclic data exchange was explained, refer section 3.3.3. Within this PROFINET operation, the parameters for cyclic data exchange such as transmission frequency, data length, specification of input/output data, etc are transmitted to the Device by the Controller. This information is utilized to extract process payload bytes from PNIO frames in input/output direction. Analysis of extracted payload bytes
from different *connections/sub-processes* to interpret underlying process behaviour as its spatio-temporal characteristics is the addressed research problem of this chapter. In particular, the spatio-temporal characteristics extraction and modeling at different granularities of sub-process (connection between Controller and Device) and process (industrial process with all connections). The research problem can be reformulated as following question:

1. How to model *spatial* characteristics of industrial (A) sub-process and (B) process? [*Addressed in section 4.3*]
2. How to model *temporal* characteristics of industrial (A) sub-process and (B) process? [*Addressed in section 4.4*]
3. How to combine *spatial* and *temporal* characteristic models of industrial (A) sub-process and (B) process? [*Addressed in section 4.5*]

### 4.2 Payload Bytes Profiling

The quest of learning the discrete process behaviour of an industrial system from its network traffic begins with outlining the requirements and assumptions made for the analysis. Then the framework for capturing the *spatial* and *temporal* characteristics of an industrial process is outlined.

#### 4.2.1 Requirements

The process data needs to be extracted from payloads of network packets. Even though the industrial protocols are not encrypted, the process data being transferred and its values within the payload are unknown to a process semantics-agnostic sniffer. Modbus protocol is an exception to the restriction on interpreting process values from network traffic for analysis. In particular, Hadžiosmanović et al. [Had14] extracted the process variables from the Modbus traffic for process analysis-based threat detection. Within the PROFINET environment, GSD files of PROFINET device provided by the manufacturer
contain information on which modules contain which device-specific physical parameters and at what positions of the payload (refer section 3.3). In a self-learning scenario, access to GSD files is not at the disposal, however, the position of these process parameters within the payload and their length is exchanged during Connection Establishment handshake for input and output data exchange (refer section 3.3.3). This information is utilized to extract payload bytes containing the process values embedded within from PNIO frames.

In addition, through Connection Establishment operation, which PROFINET component is the Controller and which is the Device is known, as Controller always initiates PN-CM handshake. For example, consider component A sending Connect request frame to component B. After successful Connection Establishment operation, A is designated as the Controller and B as the Device.

In the traffic captured from the Festo Demonstrator (refer chapter 2), 5 Controller~Device connections were found: PLC-1~Turntable-Motor, PLC-1~BK-1, PLC-2~BK-2, PLC-3~Lift-Motor and PLC-3~BK-3. The extracted process bytes from payload for output (Controller→Device) and input (Controller←Device) data exchanges are stored with corresponding timestamps.

As already mentioned in chapter 2, before the demonstrator is brought into production, referencing is done to bring the system components at their initial states of industrial process. In the captured process data, the data points of ‘referencing’ are explicitly distinguished from ‘actual process’.

### 4.2.2 Assumptions

For a discrete industrial process, the Controller is hypothesized to send a finite set of process parameters to the Device periodically at deterministic intervals with jitter. The Device communicates its dynamic process values which either varies in case of Motion Drives/Motor or remains finite in case of Bus Couplers, as observed in the demonstrator. As the output process data exchange is relatively consistent to input data, only the output process data exchange is henceforth considered for modelling the spatio-temporal characteristics of industrial process.
4.2.3 Framework

The representation of network traffic as a String, either payload information or network information, for intrusion detection has been explored by PAYL [Wan04], POSEIDON [Bol06], Anagram [Wan06] and McPAD [Per09]. These frameworks analyse payload content of each packet for positional variations at a time. However, they do not correlate the order of packets in the traffic or the duration between the transmission of different packets, which define the spatio-temporal characteristic of industrial process.

To represent the finite set of payload bytes of the process/sub-process and to characterise their spatial and temporal behaviour, a framework is proposed to encode (i) network traffic as sequence of alphabet-encoded process payload bytes, and (ii) interval between payload transitions. Since the payload bytes of process/sub-process are being profiled, the framework is called Payload Bytes Profiling (PBP).

The spatial characteristic of process/sub-process is represented by sequences of alphabet-encoded payload bytes, where the change from one alphabet to neighbouring alphabet represents a transition in process/sub-process state. The time duration between the transitions represents the temporal characteristic of the process/sub-process. The transition profile is a substring extracted from encoded traffic consisting of ordered set of alphabet-encoded payloads representing recurring transitions of the process/sub-process cycle. The intervals between the transitions of transition profile defines the interval profile for the modeled process/sub-process.

Following are the steps in creation of Payload Bytes Profile for a connection (sub-process) explained with example of PLC-1~Turntable-Motor:

(a) Payload Bytes Extraction. Using the position and length of process parameter set during Connection Establishment operation, the payload bytes are extracted from PNIO frames in output and input data exchange, as shown in fig. 4.1. As reasoned before, only the output direction is being considered further.
4.2 Payload Bytes Profiling

Figure 4.1: Process payload bytes extraction between PLC-1 and Turntable-Motor from PNIO frames (Wireshark snippet), using parameters extracted from the Connect frame.

(b) Payload Bytes Encoding. The payload bytes are converted to hexstring or bitstring representation, depending on the length of the payload bytes. The payload byte of length <1 is considered to be encoded as bit-level process parameters, hence, the bitstring representation. Each hex/bit-string is mapped to an alphabet from the English language, as shown in fig. 4.2. If the number of finite hex/bit-string surpasses 26, a new encoding scheme could be used, which remain consistent across the framework.

Figure 4.2: Alphabet-encoding of payload hexstring of sub-process PLC-1~Turntable-Motor.
(c) **Network Traffic Encoding.** The timestamped payload bytes extracted are ordered in their occurrences and encoded with corresponding alphabet encodings. In fig. 4.3, the complete encoded traffic for a sub-process *PLC-1~Turntable-Motor* captured from the demonstrator is shown.

![Encoded Traffic](image)

**Figure 4.3:** Alphabet-encoded network traffic of sub-process *PLC-1~Turntable-Motor.*

(d) **Transition Interval Computation.** The transition interval between transitions is computed as the number of timestamps before the observed payload byte, A, changes to another, B, as shown in fig. 4.4. The transition intervals for all the observed transitions of a sub-process in the traffic are collected and saved for later temporal modeling.

![Transition Intervals](image)

**Figure 4.4:** The demonstration of encoding the transition intervals from encoded traffic.

(e) **Transition Profile Extraction.** The transition profile for a sub-process is extracted from analysing it spatial characteristics, which is presented in section 4.3.

(f) **Interval Profile Extraction.** The interval profile is the result of temporal characteristics modeling of all the constituent transitions of transition profile of the sub-process, explained in section 4.4.

Additionally, the different encoded payload bytes of constituent sub-processes of industrial process are collected and re-encoded with corresponding sub-process index as suffixes, as shown in fig. 4.5.
4.2 Payload Bytes Profiling

In summary, Payload Bytes Profile for Connection X, \( P_X \), extracted from encoded process data exchange traffic, \( S_X \), for observed duration \( D_X \), can be defined as 

\[
P_X = (F_X, A_X, E_X, \Lambda_X, \Gamma^X),
\]

where

- \( S_X = (s_1, d_1), \ldots, (s_n, d_n) \), \( s_i \in A_X, s_i \neq s_{i+1} \),
- \( D_X = (d_n - d_1 + 1), d_i < d_{i+1} \), and
- \( F_X \): ‘finite’ set of payload strings (hex/bit-string) of Connection X
- \( A_X \): alphabet set s.t. \( |A_X| = |F_X| \)
- \( E_X \): encoding function, \( F_X \rightarrow A_X \) s.t.
  \[
  \forall i, j \in [1, |F_X|], \ i \neq j, a_i, a_j \in A_X : a_i \neq a_j
  \]
- \( \Lambda_X \): ordered alphabets representing Connection X’s cyclic data, \( \Lambda_X \subseteq A_X \)
- \( \Gamma^X \): transition intervals between elements of \( \Lambda_X \),
  \[
  \forall i, j \in [1, |\Lambda_X|], j > i, \gamma_i, \gamma_j \in \Lambda_X, \Gamma_{ij} = \text{transition interval model for transition } \gamma_i \rightarrow \gamma_j
  \]
4 String-based Self-learning of Process Behaviour

In next sections, the spatial and temporal characteristic modeling methodology employed to extract transition and interval profiles of a sub-process/process’s Payload Bytes Profile is detailed. These profiles are then used in conjunction for spatio-temporal modeling of corresponding sub-process or overall industrial process of the system.

4.3 Spatial Characteristic Modeling

The spatial characteristics of an industrial process is the periodicity in process data exchange. The process parameters are sent by the Controller to the Device in a definite order cyclically. In the encoded traffic, the alphabet-encoded payload bytes follows an order, which repeats contiguously, as it can be observed in fig. 4.6 for sub-process PLC-1~Turntable-Motor. Transitions between the payload bytes occur in the order: F→G, G→H, H→I, I→J, J→K, K→L, L→M, M→N, N→F, and repeat. The transition profile for this sub-process is FGHIJKLNM, and extracting such transition profile from encoded traffic of a sub-process/process requires string-based algorithms. An efficient string-based algorithm is required that extracts the transition profile over a large text.

String Basics. For the ease of exploring the string-based algorithms, certain definitions need to be established. Consider a string $S$ of length $n$ over an alphabet $\mathcal{A}$ with size $|\mathcal{A}| = \sigma$. A substring of $S$, $S[i..j]$, denotes all characters of $S$ starting index $i$ and ending at index $j$ of $S$, for $i \leq j$. The substring $S[0..i]$ denotes a prefix of $S$ of length $(i−1)$, and the substring $S[i..n-1]$ is the $i$-th suffix of $S$, denoted by $S(i)$. For example, given string $T=\text{ABCDDBCDB}$, $|T| = 8$, $T[0..4]=\text{ABCD}$ is the prefix and $T(3)=T[3..7]=\text{DBCDB}$ is the 3-rd suffix.

The transition profile extraction can be reformulated as finding the longest repeating and non-overlapping substring (LRS) from the encoded traffic. For example, for $T$, the LRS is ‘BCD’ repeating 2 times i.e. A $\underline{\text{BCD}}$ $\underline{\text{BCD}}$ B.
Dynamic Programming. With Dynamic Programming, the LRS for a string of length \( n \) can be found in \( \mathcal{O}(n^2) \) time complexity. As outlined in listing 4.1, for a given input string \( s \), a 2-dimensional array is initialized with zeros. Whenever the characters of two substrings match, their indices are saved. To avoid overlapping substrings, the length of LRS should be less than the difference between indices of substrings. The LRS is found by taking the maximum value from 2-dimensional array and the ending index of suffix. Building of 2-dimensional array takes \( \mathcal{O}(n^2) \) time, hence the similar overall complexity. The process of finding the LRS of string \( T \) is shown in fig. 4.7.

**Figure 4.6:** Spatial Characteristics of sub-process PLC-1-Turntable-Motor.
4 String-based Self-learning of Process Behaviour

Figure 4.7: The demonstration of extracting Longest Repeated and Non-Overlapping Substring (LRS) using Dynamic Programming.

Listing 4.1: The Dynamic Programming for LRS extraction.

```
1 Input String: s
2 Output String: p
3
4 n = len(s)
5 # Matrix to store values
6 m = [[0 for i in range(n + 1)]
7     for j in range(n + 1)]
8
9 p = "" # Output
10 p_len = 0 # Length of output
11
12 suffixEndIndex = 0
13 for i in range(1, n + 1):
14     for j in range(i + 1, n + 1):
15         # m[i-1][j-1] < (j-i) to avoid overlapping
16         if (s[i - 1] == s[j - 1] and m[i - 1][j - 1] < (j - i)):
17             m[i][j] = m[i - 1][j - 1] + 1
18
19         # updating maximum length of the substring
20         # and updating the ending index of the suffix
21```
Suffix Tree and Regular Expression Search. The search for an efficient string-based algorithm over a large text in comparison to Dynamic Programming, found its nest in the field of Computational Biology, in particular Genomics. Genomics is analysis of the genome of an organism, a biological sequence of Deoxyribonucleic acid (DNA), Ribonucleic acid (RNA) or proteins, to find related ancestors (phylogenetics), repeated segments containing functional information and their mutations (genetics) and many more biological properties. A genome is usually very large in size, for example, human genome is up to 3.2 billions base pair (base pair = [A, T, G, C]) [Col03]. Dan Gusfield [Gus97] described different data structures and algorithms for string manipulations on such larger text, such as suffix tree, suffix array, etc. Amongst them, Suffix Tree has been widely used in biological sequence analysis tasks such as finding tandem repeats, which are repeated segments appearing adjacent to each other. The other applications of Suffix Tree are in exact string matching, data compression, longest repeated substring search, etc [Abo09].

Suffix Tree was introduced by Pete Weiner, in 1973 [Wei73], with linear construction time $O(n)$ for a string of length $n$. McCreight, in 1976 [McC76], and Ukkonen, in 1995 [Ukk95], have incrementally improved on the space-complexity of constructing a suffix tree in linear time. In particular, Ukkonen’s is an on-line algorithm, where the whole string doesn’t have to be read and stored at once, and is easy to understand.
Figure 4.8: The demonstration of extracting Longest Repeated Substring using Suffix Tree.
A suffix tree for a string $S$ of length $n$ is a rooted directed tree such that:

- It has exactly $n$ leaves numbered from 1 to $n$.
- Except the root, each interval node has at least two children.
- Each edge is labelled with a non-empty substring of $S$.
- No two outgoing edge-labels from a node begin with same character.
- For any leaf $i$, the $i$-th suffix is constructed by concatenating edge-labels on the path from root to leaf $i$ i.e. $S[i .. n]$, for $1 \leq i \leq n$.
- For any non-leaf node $k$, concatenation of edge-labels on the path from root to $k$ is substring $S[1 .. k]$ as its path label, and occurs $z$ times, where $z$ is the number of leaves in the subtree of node $k$.
- For any non-leaf node $k$ with path label $ap$, where $a$ is a character and $p$ is a string, a suffix link is a pointer from $k$ to another node whose path label is $p$.

In fig. 4.8, a suffix tree for string $T=ABCDBCDB$ is shown. Every string is appended with the terminal character, $\$$, to ensure that no suffix is prefix of another, and every suffix belongs to a leaf. For example, for a string $PP$, without the terminating character, the second suffix, which is a prefix of the first, won’t find its place at the leaves of the suffix tree. Additionally, for linear space complexity, each edge-label, a substring of $S$, $S[i .. j]$ is replaced with a pair of position indices $(i, j)$.

In order to find the longest repeated substring in string $S$ with a suffix tree, we search for the deepest internal node of the suffix tree and its path label is the solution [Sun09]. Such is the case because for a substring repeating at $i$ and $j$ positions in $S$, it has to be the common prefix of $i$-th suffix and $j$-th suffix. Hence, the longest repeated substring is found at the deepest internal node. As the suffix tree has at most $n$ nodes, the traversal to find the deepest takes $O(n)$ time. For our example string $T$, the longest repeated substring is BCDB, as shown in fig. 4.8.
The longest repeated substring search with suffix tree is linear in time in comparison to quadratic Dynamic Programming solution. However, the caveat with the suffix tree’s solution is that it retrieves the longest repeated overlapping substring. In order to extract the non-overlapping string, a regular expression (RegEx) search is made recursively in linear time [Cox07]. At every step, the RegEx: `^\w*\1\$`, finds the word group which is the suffix and prefix of the string, then it is sliced off from the end of the string. It is performed recursively until no more such word group can be found and the word group is returned as the non-overlapping repeating substring. For the output of suffix tree search, BCDB, the non-overlapping substring is BCD, which occurs 2 times in the input string T i.e. `A BCD BCD B`.

The longest repeating non-overlapping string of length \(m\) from a string of length \(n\) can be extracted from a string’s suffix tree with additional RegEx operation in linear operations of \(O(n + k \times m)\), where \(m < n\) and it repeats at least \(k\) times, for \(2 \leq k \leq \frac{n}{k}\). The overall algorithm is outlined in listing 4.2 which is further used for transition profile extraction from the encoded traffic.

```plaintext
# Listing 4.2: The RegEx-coupled Suffix Tree algorithm to extract LRS.

1. Input String: s
2. Output String: p
3. T = Build_SuffixTree(s)
4. T.doDepthFirstTraversal()
5. d = T.deepestInternalNode()
6. # Longest Repeated Substring
7. lrs = T.getPathLabel(T.root(), d)
8. # RegEx
9. p = Get_NonOverlapping_String(lrs)
```

The RegEx-coupled Suffix Tree algorithm is employed to extract transition profile for all the sub-processes. An example is outlined in fig. 4.9 to demonstrate the transition profile extraction for sub-process `PLC-1~Turntable-Motor`, resulting to `FGHIJKLMN`, as it was expected at the beginning of the section.
Figure 4.9: The demonstration of extracting Transition Profile of sub-process PLC-1-Turntable-Motor using Suffix Tree.
The *transition profile*, FGHJKLMN, is used to (a) check if the order of transitions are being followed in the traffic, and (b) distinguish payload bytes outside the sub-process and flag their occurrences. In fig. 4.10, the payloads and the transitions outside the *transition profile* are flagged as ‘invalid transitions’, represented with red coloured line. The red line at the beginning corresponds to ‘referencing’ phase of the demonstrator, where the process values other than the ones constituting the ‘actual process’ are transmitted. This difference in process data exchange at different phases is clearly distinguishable using the *transition profile*.

![Encoded Traffic](image)

**Figure 4.10:** Classification of transitions as Valid or Invalid using Transition Profile of sub-process PLC-1-Turntable-Motor - FGHJKLMN.

The RegEx-coupled Suffix Tree algorithm is applied over the encoded traffic of the process and ‘valid/invalid transitions’ are detected, as shown in fig. 4.11. The red line at the beginning corresponds to ‘referencing’ phase of the demonstrator and only partial encoded traffic from the beginning is shown for brevity.
4.3 Spatial Characteristic Modeling

Figure 4.11: Classification of transitions as Valid or Invalid using Transition Profile of the Festo Demonstrator’s process.
4.4 Temporal Characteristic Modeling

The temporal characteristics of an industrial process is the deterministic intervals between the process data exchanges. At their core, the industrial processes are characterized by their deterministic time requirements, which required customized industrial protocols to satisfy them. Modeling the temporal characteristics contributes toward detecting subtle changes of the industrial process at fine-granularity level. A classifier is trained on transitioning time intervals between process parameter, sent from the Controller to the Device, collected during the “normal” operation of industrial process. Whenever the transition interval deviates from learned temporal characteristics, the classifier classifies it as an anomaly (or an outlier).

![Temporal Characteristic Modeling Diagram](image)

**Figure 4.12:** Temporal Characteristics of sub-process PLC-1-Turntable-Motor: intervals for every transition in transition profile.
For a sub-process/process, the transition intervals between payload bytes constituting its transition profile are modeled by set of classifiers, each for a transition, and collectively constitutes interval profile of the sub-process/process. As an example, for sub-process PLC-1~Turntable-Motor, the transitions between payload bytes of its transition profile (FGHIJKLMNOP) are FG, GH, HI, IJ, JK, KL, LM, MN, AND NF, and their corresponding transition intervals for the encoded traffic are shown in fig. 4.12. The ‘referencing’ and ‘actual process’ phases data points are differentiated as shown in the figure.

4.4.1 Model Selection

The selection of classifier for interval profile needs to satisfy following criteria:

- **Non-parametric method.** The transition intervals are collected in a self-learning environment where no prior information about the data is available. The parameters of the model are not foreseeable and are not fixed. Non-parametric methods are robust and employed in such scenarios, hence, the required classifier must be non-parametric.

- **Univariate analysis.** Only the interval feature is being model, therefore, the classifier must perform well on univariate data.

- **One-class classification.** The transition intervals are collected from the normal operations of the industrial process. All the collected data points belong to one class “normal”. One-class classifiers that learn on a particular class and detect anomalies/outliers deviating from the learnt one-class features. Hence, the classifier must be an on-class classifier.

Based on above criteria, density-based Local Outlier Factor (LOF), boundary-based One-Class Support Vector Machines (OC-SVM) and tree-based Isolation Forest (IF) methods are selected. They have been widely used for anomaly/outlier detection in research as well as real-world applications with efficient performances [Pol22]. In addition, for a self-learning system, analysing the problem from different perspective brings in-depth insights.
4.4.1.1 Local Outlier Factor

Local Outlier Factor (LOF) is a density-based anomaly detection algorithm that compares density of a given data point to its neighbours to determine if its anomalous or not. The anomalous points are hypothesized to lie in lower density regions as compared to populous normal points. The idea of LOF was proposed by Breunig et al. [Bre00] to find anomalous points by calculating the local deviation of a given data point to its neighbouring points. The settings and process of calculating LOF of a data point \( p \) i.e. \( LOF(p) \) are defined as follows:

**k-distance & k-neighbours.** The distance between point \( p \) and point \( o \), where \( o \) is \( p \)’s \( k \)-th nearest neighbour, defines \( k \)-distance of \( p \) i.e. \( kd(p) \). All the points that are in neighbourhood of \( p \) at distance less than \( kd(p) \) are its \( k \)-neighbours i.e. \( N_{kd}(p) \).

**Reachability distance.** The *reachability distance* of point \( p \) to point \( o \), \( reachdist_{kd}(p,o) \), is the maximum of distance from \( o \) to \( p \) and \( k \)-distance of \( o \). In other words, if \( p \) is in \( k \)-neighbours of \( o \) \( (N_{kd}(o)) \), then reachability distance is \( k \)-distance of \( o \) \( (kd(o)) \), otherwise its actual distance between them \( d(p,o) \).

\[
reachdist_{kd}(p,o) = \max\{kd(o), d(p,o)\}
\]

**Local reachability density.** The *local reachability density* of point \( p \), \( LRD_{kd}(p) \), is the inverse of the mean of reachability distance of \( p \) from its neighbours. Intuitively, the lower the \( LRD_{kd}(p) \), the less dense the \( p \)’s neighbourhood and thus longer to reach its neighbourhood points.

\[
LRD_{kd}(p) = \frac{1}{\sum_{o\in N_{kd}(p)} \frac{reachdist_{kd}(p,o)}{|N_{kd}(p)|}}
\]

**Local outlier factor.** The *local outlier factor* of \( p \), \( LOF_{kd}(p) \), is the ratio of average local reachability density of its neighbours to its own local reachability density. Intuitively, if \( p \) is an *inlier*, the average LRD of its neighbours is same
as the $LRD_{kd}(p)$, amounting the ratio to 1. Otherwise, the point $p$ is an outlier with high LOF score.

$$LOF_{kd}(p) = \frac{\sum_{o \in N_{kd}(p)} LRD_{kd}(o)}{|N_{kd}(p)|} \times \frac{1}{LRD_{kd}(p)}$$

### 4.4.1.2 Isolation Forest

Isolation Forest (IF), proposed by Liu et al. [Liu08], is an ensemble of optimized binary trees (iTrees), where the data points are recursively partitioned until all the instances are isolated. The data instance with shortest average path from root is the anomalous point. The intuition behind this is that the anomalies are “rare” as compared to normal points resulting in fewer partitions, hence, shorter path in tree.

For a dataset with $n$ instances, an Isolation Forest is built by creating multiple iTrees, each recursively partitioning the data points until all $n$ instances are isolated. For each data instance $x$, $h(x)$ is its path length measured as the number of edges traversed from root to $x$ in an iTree. It is normalized with the average path length $c(n)$. Liu et al. observed that an iTree is similar to Binary Search Tree (BST) and the value of $c(n)$ can be thought of as path length of unsuccessful search in the BST. The value of $c(n)$ is calculated based on following equation, where $H(i)$ is the harmonic number, which can be estimated by $\ln(i) + 0.5772156649$ (Euler’s constant):

$$c(n) = 2H(n - 1) - \left(\frac{2(n - 1)}{n}\right)$$

The anomaly score for each data instance $x$ is calculated as

$$s(x,n) = 2\frac{-E(h(x))}{c(n)} ,$$

where $E(h(x))$ is the average path length of $x$ from a collection of iTrees. An anomaly score of 0 indicates $x$ to be normal, and closer to 1 indicates high probability of being anomalous.
4.4.1.3 One-Class Support Vector Machines

One-Class Support Vector Machines (OC-SVM), proposed by Schölkopf et al. [Sch99], are one-class classifiers derived from the SVM classifier [Bos92]. It finds a hyperplane that separates given data points of a particular class from the origin. Any new point near to the origin or on its side of hyperplane would be classified as an anomaly. The hyperplane must be positioned in such a way that it maximizes the distance between nearest sample of given class and origin, this distance is called “margin”.

When the input space is not linearly separable, it is projected to a higher dimensional feature space \( F \) where the hyperplane can separate the data points using a non-linear function \( \phi(.) \). The hyperplane is projected back to linear space and has a non-linear shape. In particular, \( K(x,x_i) = \phi(x)^T \phi(x_i) \) is called the kernel function. The most widely employed kernel functions are linear, polynomial, sigmoid, and Radial Basis Function (RBF).

To prevent the classifier from overfitting, slack variables \( \xi \) are introduced to allow some data points to lie within the margin. [Sch99] defines the regularization parameter \( \nu \) for tuning the trade-off between maximizing the margin and number of training data points to be within the margin.

The objective function of OC-SVM for minimization can be formulated as

\[
\min_{w,\xi,\rho} \left\{ \frac{\|w\|^2}{2} + \frac{1}{n\nu} \sum_{i=1}^{n} \xi_i - \rho \right\}
\]

subject to:

\[
w^T \phi(x_i) \geq \rho - \xi_i \quad \forall i, i = 1, ..., n
\]

\[
\xi_i \geq 0 \quad \forall i, i = 1, ..., n
\]

where, \( w \) is the orthogonal vector to hyperplane, \( n \) is total number of sample points, \( \xi_i \) is the slack variable, \( \rho \) is the margin. \( \nu \) is the regularization parameter that characterizes the solution: (1) sets an upper bound on fraction of outliers, and (2) is a lower bound on number of training data points as Support Vectors.
Solving the minimization problem with Lagrange Multipliers and using kernel function for dot-product calculation, the decision function for a data point \( x \) becomes

\[
f(x) = \text{sign}(w^T \phi(x) - \rho) = \text{sign}(\sum_{i=1}^{n} \alpha_i K(x, x_i) - \rho).
\]

Here, \( \alpha_i \) are the Lagrange multipliers and every \( \alpha_i > 0 \) is weighted in the decision function thus supports the machine. OC-SVMs thus create a hyperplane characterized by \( w \) and \( \rho \) with maximal distance from the origin in feature space \( F \) and separating all points from the origin.

### 4.4.2 Performance Metric

The efficiency of a classifier’s performance in detecting anomalies/outliers is governed by the choice of the evaluation metric during training phase. Choosing an incorrect metric results in poor modeling and eventually poor performance on anomaly/outlier detection. In a balanced dataset, normal (positive) and anomalies/outliers (negative) are equally distributed and confusion matrix [21a] elements, shown in table 4.1, are calculated.

<table>
<thead>
<tr>
<th>Predicted Positive</th>
<th>Predicted Negative</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Positive (P)</strong></td>
<td>True Positive (TP)</td>
</tr>
<tr>
<td><strong>Negative (N)</strong></td>
<td>False Positive (FP)</td>
</tr>
</tbody>
</table>

Different metrics are calculated from the confusion matrix:

- **Accuracy** = \( \frac{TP + TN}{TP + TN + FP + FN} \)
- **Sensitivity/Recall** = \( \frac{TP}{TP + FN} \)
- **Specificity** = \( \frac{TN}{TN + FP} \)
When the distribution of classes is highly skewed with only one class being present, standard performance metric such as Accuracy do not suffice. There are no negative classes to account for and every classifier trained on this skewed distribution gives high accuracy.

During the training of a classifier for anomaly detection on “normal” operational data, its performance is evaluated on how well it has learnt the data characteristics to recall them. Hence, Sensitivity/Recall will be used as performance metric during training.

When a skewed dataset with outliers/anomalies is being evaluated, the classifier is evaluated on how well it distinguishes anomalies/outliers from normal data points, reflected in its Specificity metric. The overall anomaly detection performance of the classifier in a skewed dataset is measured with Balanced Accuracy [Mow05] defined as

\[
\text{Balanced Accuracy} = \frac{\text{Specificity} + \text{Sensitivity}}{2}
\]

The higher the Balanced Accuracy, the better the classifier performs in distinguishing normal and outliers/anomalies.

### 4.4.3 Temporal Characteristic Modeling

For each sub-process, transition intervals of all the transition of its transition profile are modeled with OC-SVM, IF and LOF (section 4.4.1.1-section 4.4.1.3). The classifiers for transitions with these methods are implemented in a scikit-learn python-based library [Ped11]. Each method class outputs \(-1\) when an outlier/anomaly is detected, otherwise \(+1\) for inlier/normal data point. Following these observations, for a given sub-process \(Z\) and its transition \(XY\), where \(X\) payload byte transits to \(Y\) payload byte, an interval instance \(w\) is classified with \(Z\)'s interval profile constituent classifier \(\Gamma_{XY}\) as follows:

\[
\Gamma_{XY}(w) = \text{sign}(\Gamma_{XY}^{LOF}(w) + \Gamma_{XY}^{OCSVM}(w) + \Gamma_{XY}^{IF}(w))
\] (4.1)
where, $\Gamma^\text{LOF}_{XY}$, $\Gamma^\text{OC-SVM}_{XY}$ and $\Gamma^\text{IF}_{XY}$ are XY transition interval classifier with LOF, OC-SVM and IF, respectively. The $\Gamma_{XY}(w)$ value $\leq 1$ classifies the interval as an anomaly/outlier, otherwise normal.

**Hyperparameter tuning.** For each anomaly/outlier detection methodology, a grid search with cross-validation scheme is performed to get the best parameters of the methods for the optimal performance score. The score function chosen for the grid search is *Sensitivity/Recall*. Grid search exhaustively evaluates the grid of parameters provided to get the best score. In particular, for LOF, the value for number of neighbours ($k$) is tuned, as choosing a bigger neighbourhood could miss the local outliers. For OC-SVM, the *kernel function* ($\phi(.)$) appropriate for the given data set is tuned. For all the methods, the upper bound on number of allowed misclassified training data points is additionally tuned.

**Modeling with tuned hyperparameters.** The tuned hyperparameters for each anomaly/outlier detection methodology are used to model the transition intervals of a sub-process. In table 4.2, the performance metric on the training data by individual method for sub-process *PLC-1-Turntable-Motor* is presented. In certain cases, the recall is less than 100%, which results from either tuned upper bound on allowed misclassification or these misclassified data points lie in the region away from rest of the data points that methods couldn’t model.

Table 4.2: **Performance of temporal modeling methods for sub-process PLC-1-Turntable-Motor.**

<table>
<thead>
<tr>
<th>Transitions</th>
<th>OneClass SVM</th>
<th>Isolation Forest</th>
<th>Local Outlier Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>FG</td>
<td>0.98</td>
<td>0.98</td>
<td>1.00</td>
</tr>
<tr>
<td>GH</td>
<td>0.98</td>
<td>0.98</td>
<td>1.00</td>
</tr>
<tr>
<td>HI</td>
<td>1.00</td>
<td>0.98</td>
<td>1.00</td>
</tr>
<tr>
<td>IJ</td>
<td>0.98</td>
<td>0.98</td>
<td>1.00</td>
</tr>
<tr>
<td>JK</td>
<td>1.00</td>
<td>0.98</td>
<td>1.00</td>
</tr>
<tr>
<td>KL</td>
<td>0.98</td>
<td>0.98</td>
<td>1.00</td>
</tr>
<tr>
<td>LM</td>
<td>1.00</td>
<td>0.98</td>
<td>1.00</td>
</tr>
<tr>
<td>MN</td>
<td>0.81</td>
<td>0.98</td>
<td>1.00</td>
</tr>
<tr>
<td>NF</td>
<td>0.98</td>
<td>0.98</td>
<td>1.00</td>
</tr>
</tbody>
</table>
Figure 4.13: Temporal characteristic modeling of transitions in sub-process PLC-1-Turntable-Motor.
In fig. 4.13, the performance of the individual methods in detecting outliers/anomalies in the training data is shown. When the data points of ‘referencing’ phase are different from ‘actual process’ points, they are classified as “Outliers” (circled red). It is also evident from this figure that combining results from these methods is beneficial, with rare exceptions.

**Interval profile.** For each sub-process, its *interval profile* is the set of classifiers for intervals of transitions from its *transition profile*, each defined as eq. (4.1). As an example, for sub-process PLC-1~Turntable-Motor, its *interval profile* is \{\Gamma_{FG}, \Gamma_{GH}, \Gamma_{HI}, \Gamma_{IJ}, \Gamma_{JK}, \Gamma_{KL}, \Gamma_{LM}, \Gamma_{MN}, \Gamma_{NF}\}. In fig. 4.14, these are employed on the encoded traffic and classify a transition interval as ‘valid/invalid interval’. The red lines at the beginning reflects the ‘referencing’ phase where certain transition have invalid intervals as compared to ‘actual process’. This difference in the transition intervals can be observed in the figure too. There are intervals misclassified amounting to 2/3 of constituting anomaly/outlier detection methods misclassifying these intervals.

**Figure 4.14:** Classification of transition intervals as *Valid* or *Invalid* using *Interval Profile* of sub-process PLC-1~Turntable-Motor.
The *interval profile* is also applied over the transition intervals of process and *valid/invalid* transition intervals are detected, as shown in fig. 4.15. The red line at the beginning corresponds to the ‘*referencing*’ phase of the demonstrator and only partial encoded traffic from the beginning is shown for brevity.
4.4 Temporal Characteristic Modeling

Figure 4.15: Classification of transition intervals as Valid or Invalid using Interval Profile of the Festo Demonstrator’s process.
4.5 Spatio-temporal Characteristic Modeling with Payload Byte Profiling

The spatial and temporal characteristics of an industrial process and its constituent sub-processes are captured in the transition profile and interval profile of their Payload Byte Profiles. For spatio-temporal characteristic modeling, their transition and interval profiles are combined to score a payload byte transition. For a sub-process $Z$, a transition instance $t_{XY}$ of $Z$’s transition XY with $d$ seconds transition interval, where X payload byte transits to Y payload byte in $Z$, has the profile score $\Theta_{XY}^{Z}$ as follows:

$$\Theta_{XY}^{Z}(t_{XY}, d) = \text{sign}(\Lambda_{Z}(t_{XY}) + \Gamma_{XY}^{Z}(d)) \quad (4.2)$$

such that, $\Lambda_{Z}(t_{XY}) = \begin{cases} +1 & \text{if valid transition} \\ -1 & \text{otherwise} \end{cases}$

$\Gamma_{XY}^{Z}(d) = \begin{cases} +1 & \text{if valid interval} \\ -1 & \text{otherwise} \end{cases}$

where $\Lambda_{Z}$ is $Z$’s transition profile, and $\Gamma_{XY}^{Z}$ is the constituent classifier for transition XY in $Z$’s interval profile. The profile score of $-1$ marks the transition instance invalid or anomalous, otherwise normal.

A transition instance which follows the order with incorrect transition duration would be flagged valid by the transition profile. Combining interval profile for the overall decision would correctly classify it as an anomaly. The advantage of such a combination can be observed in fig. 4.16, where transitions of sub-process PLC-1-Turntable-Motor are evaluated for spatio-temporal characteristics using eq. (4.2). The red lines at the beginning correspond to ‘referencing’ phase and it can be observed how interval profile is correcting transition profile’s incorrect classification.
The spatio-temporal characteristic modeling with PBP is also applied to the overall process and every transition is classified as normal/anomaly, as shown in fig. 4.17. The red line at the beginning corresponds to the ‘referencing’ phase of the demonstrator and only partial encoded traffic from the beginning is shown for brevity.
Figure 4.17: Classification of transitions as Normal or Anomaly using Transition Profile and Interval Profile of the Festo Demonstrator’s process.
4.6 Discussion and Summary

4.6.1 Production Cycle Detection of Festo Demonstrator

The production cycle of an industrial process is defined by the deterministic and periodic execution of process parameters in constituent sub-processes. In every production cycle, a product is either newly produced or processed for enhancements as is the case with the Festo Demonstrator (refer chapter 2). Detecting the production cycle from the network traffic provides information that could be used for quantifying process throughput or optimization of the process utilizing timing information [Bun20].

In the PBP framework, the production cycle of an industrial process is its transition profile extracted from its encoded traffic. The framework is employed on the Festo Demonstrator’s process to encode the traffic (refer fig. 4.5) and extract its transition profile:


For interpretation of the extracted process’ transition profile as its production cycle, the foundations of PROFINET operations from chapter 3 are reiterated and utilized. Within output data exchange, every process payload byte contains process parameters sent from the Controller to the Device. Using the engineering tool, the process payload bytes are mapped to process events engineered during System Engineering PROFINET operation (refer section 3.3).
Furthermore, in fig. 4.18, the *Festo Demonstrator*’s devices and auxiliary process event information are highlighted in yellow colour. For *Turntable*, the different positions on the storage (1-8) are marked. The direction of *Upper Band* and *Lower Band*, and *Lift*’s position at the bottom (*LiftReset*) and the top (*LiftUp*) are shown. The associated information of *Gripper*, *Upper Piston* and *Lower Piston* are not shown for brevity. The complete mapping of encoded process payload bytes to corresponding process event instructions is summarized in table 4.3.
Table 4.3: Summary of the Festo Demonstrator’s payload bytes mapped to engineered process events.

<table>
<thead>
<tr>
<th>Sub-Process</th>
<th>Alphabet-Encoded Payload</th>
<th>Engineered Process Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLC-2~BK-2</td>
<td>A1</td>
<td>BandReset</td>
</tr>
<tr>
<td></td>
<td>B1</td>
<td>MoveUpperBand_CloseBarrier</td>
</tr>
<tr>
<td></td>
<td>C1</td>
<td>MoveLowerBand</td>
</tr>
<tr>
<td>PLC-1~Turntable-Motor</td>
<td>F2</td>
<td>TurntablePosition01</td>
</tr>
<tr>
<td></td>
<td>G2</td>
<td>TurntablePosition02</td>
</tr>
<tr>
<td></td>
<td>H2</td>
<td>TurntablePosition03</td>
</tr>
<tr>
<td></td>
<td>I2</td>
<td>TurntablePosition04</td>
</tr>
<tr>
<td></td>
<td>J2</td>
<td>TurntablePosition05</td>
</tr>
<tr>
<td></td>
<td>K2</td>
<td>TurntablePosition06</td>
</tr>
<tr>
<td></td>
<td>L2</td>
<td>TurntablePosition07</td>
</tr>
<tr>
<td></td>
<td>M2</td>
<td>TurntablePosition08</td>
</tr>
<tr>
<td></td>
<td>N2</td>
<td>TurntablePositionReset</td>
</tr>
<tr>
<td>PLC-3~Lift-Motor</td>
<td>F3</td>
<td>LiftPositionReset</td>
</tr>
<tr>
<td></td>
<td>G3</td>
<td>LiftPositionUp</td>
</tr>
<tr>
<td>PLC-1~BK-1</td>
<td>A4</td>
<td>GripperReset</td>
</tr>
<tr>
<td></td>
<td>B4</td>
<td>GripperPush</td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td>GripperDown</td>
</tr>
<tr>
<td></td>
<td>D4</td>
<td>GripperClose_Up</td>
</tr>
<tr>
<td></td>
<td>E4</td>
<td>GripperClose_Pull</td>
</tr>
<tr>
<td></td>
<td>F4</td>
<td>GripperClose_Down</td>
</tr>
<tr>
<td></td>
<td>G4</td>
<td>GripperClose</td>
</tr>
<tr>
<td></td>
<td>H4</td>
<td>GripperUp</td>
</tr>
<tr>
<td>PLC-3~BK-3</td>
<td>B5</td>
<td>LowerPistonPull</td>
</tr>
<tr>
<td></td>
<td>C5</td>
<td>LowerPistonPull_UpperPistonPush</td>
</tr>
<tr>
<td></td>
<td>D5</td>
<td>LowerPistonPush</td>
</tr>
<tr>
<td>PLC-1~PLC-3</td>
<td>E6</td>
<td>LiftStay</td>
</tr>
<tr>
<td></td>
<td>F6</td>
<td>MoveLift</td>
</tr>
<tr>
<td>PLC-1~PLC-2</td>
<td>C7</td>
<td>BandStay</td>
</tr>
<tr>
<td></td>
<td>D7</td>
<td>MoveBand</td>
</tr>
</tbody>
</table>
Figure 4.19: The Festo Demonstrator’s production cycle detected with PBP.
Using the table 4.3 on the extracted process’ transition profile, as its production cycle, the order of process events at every timestep is represented in fig. 4.19. The detected production cycle has been confirmed as correct by the Engineer of the Festo Demonstrator’s automation project. It can be visually verified from fig. 4.19, the order of instructions sent from the Controller are same as process description in chapter 2:

1. **Gripper** to pick up a *piece* from **Turntable** (GripperDown→GripperClose_Up), and put down on the **Upper Band** (GripperClose_Pull→GripperClose_Down→GripperClose→GripperUp→GripperReset)

2. **Upper Band** to move while closing the barrier to slide down the *piece* to **Lower Band** (MoveUpperBand_CloseBarrier). Then, to move **Lower Band** to put the *piece* on Lift’s platform (MoveLowerBand→BandReset).

3. **Lift** to move the *piece* to the top followed by **Upper Piston** to push it into the **Stock** (LiftPositionUp→LowerPistonPull_UpperPistonPush).

4. **Lower Piston** to push the *piece* onto the **Turntable** out of the **Stock** (LowerPistonPush), and **Lift** to drive back to bottom (LiftPositionReset→LowerPistonPull).

5. **Turntable** to rotate to new position (TurntablePosition01), and **Gripper** to move out onto the **Turntable** (GripperPush).

6. 1-5 are repeated for all of the Turntable’s positions (TurntablePosition01, ..., TurntablePosition08), and restarts the production cycle with resetting the Turntable’s position counter (TurntablePositionReset).

### 4.6.2 Anomaly Detection with Payload Byte Profiling

An adversary, with the knowledge of process parameters and employed industrial components, could either change the process parameters or the component configurations. For the Festo Demonstrator use case, a ‘Force Attack’ changes the process parameters of the Lower Band to move it in reverse direction chapter 2. The additional attack scenario, ‘Rename Attack’, changes the logical name of the Turntable-Motor to make it inaccessible to other device
within the process. Detection of such attacks through process data analysis is evaluated with the PBP framework, and its qualitative comparison to detection performance of a commercial NIDS is made.

The network traffic from the Festo Demonstrator with simulated attacks is captured and used for the analysis. Through PBP, the ‘Force Attack’ was easily detected as it did not suffice the already learnt transition profile for the Demonstrator’s process. In fig. 4.20, the anomalous instance and corresponding process payload byte is pointed with an arrow. The horizontal dashed line shows the invalid transition, interval and overall anomaly classification of this event in the traffic.

**Figure 4.20:** The demonstration of anomaly detection using PBP.
4.6 Discussion and Summary

Table 4.4: The anomaly detection performance of Payload Bytes Profiling (PBP).

<table>
<thead>
<tr>
<th></th>
<th>Overall</th>
<th>Normal</th>
<th>Force Attack</th>
<th>Rename Attack</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensitivity</td>
<td>0.97</td>
<td>0.97</td>
<td>0.85</td>
<td>1.00</td>
</tr>
<tr>
<td>Specificity</td>
<td>0.77</td>
<td>0.00</td>
<td><strong>1.00</strong></td>
<td>0.00</td>
</tr>
<tr>
<td>Balanced Accuracy</td>
<td>0.63</td>
<td>0.49</td>
<td>0.93</td>
<td>0.50</td>
</tr>
</tbody>
</table>

In table 4.4, the overall performance for anomaly detection on the collected data is summarized. With the framework, 97% of the normal packets were correctly recalled and 77% of the anomalous instances were detected, from table’s first column. To evaluate the performance at finer granularity, the Specificity and Sensitivity were calculated for normal and two attack traffic packets. The ‘Force Attack’ as already mentioned is correctly classified as anomalous, however, ‘Rename Attack’ packets were not detected at all. In the ‘Rename Attack’, only the device property is being manipulated not the process, hence, no change in process bytes exchanged in output direction.

The collected traffic is analysed through a commercial NIDS which successfully detected ‘Rename Attack’, but couldn’t detect the change in the process payload bytes sent in ‘Force Attack’. The NIDS is a rule-based system which utilizes protocol-based and traffic mining information to detect anomalies. Its anomaly detection capability on process information could be enhanced with integration of the PBP framework.

Through successful detection of ‘Force Attack’, the PBP framework satisfies the BSI’s “Category D - unusual changes in process data” requirement, outlined in section 1.1.1, for detecting anomalies in an industrial process.
4.6.3 Review

For a string of length $n$ and alphabet $\mathcal{A}$, the space complexity of its suffix tree is $O(n|\mathcal{A}| \log n)$. In 1993, Udi Manber and Gene Myers [Man93], introduced Suffix Array as a data structure to store suffixes of a string in a lexicographically increasing order. It has $O(n \log n)$ space complexity and is independent of alphabet size. The longest repeated string is found by comparing neighbouring suffixes for ‘Longest Common Prefix (LCP)’ and the LCP with largest size is returned. This has overall runtime complexity of $O(n \log n)$ for a string of length $n$ [Sun09]. When there is no restriction on runtime and string is quite large in size, a suffix array could be substituted for a suffix tree in section 4.3.

One-Class Support Vector Machines are better at detecting global outliers in data than local outliers. This gap is filled by Local Outlier Factor and Isolation Forest, and together all three methods cover the whole range of outliers. However, the quality of data used in their training is the decisive factor on their anomaly/outlier detection performance. If it contains noise then the methods would learn false positives instances as normal. In section 4.4.3, the data is assumed to be devoid of unwanted noise. In industrial networks, an application-specific acceptable jitter/noise in transition intervals is allowed, which is included for the analysis as part of normal operations.

The PBP framework has been conceptualized with PROFINET as an instance of industrial network protocol. Nevertheless, it is extensible to any industrial protocol in discrete process as the requirements (refer section 4.2.1) and spatio-temporal characteristics remain same. For an industrial protocol $\mathcal{E}$, a protocol dissector is required that extracts payload bytes containing process parameters from process data exchanges utilizing $\mathcal{E}$. The rest of the procedure to extract the interval and transition profiles of underlying process follows as described in section 4.3 and section 4.4.

Bunte et al. [Bun20] presented an automaton based approach to detect production cycle in production plants. The employed automaton, Online Timed Automaton Learning Algorithm (OTALA), keeps track of number of passes through different sets of state transitions. Each state consists of all discreet
value the system, and transitions are triggered by change in discrete signals. The PBP framework also considers change in signals (process parameters), captured in alphabet-encode process payload bytes. It detects the production cycle in linear time and doesn’t keep a history of different transition matrices as the OTALA-based algorithm. Both the methods operate on similar information i.e. change in signals with different approaches to arrive at same goal of production cycle detection.

The ‘Force Attack’ on the Festo Demonstrator sends new process parameters in the output data exchange, triggering the change in spatial characteristics of sub-process PLC-2~BK-2, hence, detected easily using its transition profile. Korkmaz et al. [Kor17] presented time delay injection attack in ICS, where an attacker injects extra extra time delays in the underlying process to cause anomalous operational regime, leading to system crash. The time delays are introduced incrementally at lower rate to avoid detection by system devices. This gradual increase in the time delays would be detected as invalid transition intervals using the interval profile of the underlying process. Implementing such attacks need precision in intercepting the traffic at right moment and injecting right amount of time delays. Collection of these configurations on the Festo Demonstrator is ongoing and a similar attack will be added for evaluating PBP framework’s capability in its detection.

4.6.4 Conclusion

In this chapter, the extraction of spatio-temporal characteristics of an industrial process from its network traffic for process behaviour analysis in a self-learning setup is addressed. A framework, Payload Bytes Profiling (PBP), capturing the spatial and temporal characteristics of an industrial process, and its constituent sub-processes, through alphabet-encoding of process payload bytes is introduced. The transition profile representing the spatial characteristic is extracted with RegEx-couple Suffix Tree based algorithm in section 4.3. The temporal characteristic is the interval between transitions of transition profile, and is modeled as set of classifiers, one for each transition pair, in section 4.4. The classifier inherently constitutes of density-based Local Outlier
Factor, boundary-based One-Class Support Vector Machines and tree-based Isolation Forest anomaly/outlier detection classifiers in combination for detecting valid/invalid transition interval.

The PBP framework in section 4.6.1 has been used to detect the production cycle of the Festo Demonstrator, which has been verified by the Engineer of the Demonstrator’s automation project. In section 4.6.2, the PBP framework’s role as a process analysis-based IDS in successfully detecting a process-targeted attack, ‘Force Attack’, on the Demonstrator is outlined. Thus satisfying the BSI’s “Category D - unusual changes in process data” requirement of an anomaly detection system to detect anomalies in an industrial process, as outlined in section 1.1.1. In conclusion, the PBP framework is extensible to any industrial protocol in discrete process as the requirements and spatio-temporal characteristics remain same.

In the next chapter, the research problems associated with analysing the PNIO frames for anomaly detection of industrial process behaviour through Graph Representation Learning is being addressed.
5 Graph-based Self-learning Process Behaviour from Network Traffic

A Graph is an ubiquitous representation of systems where the interactions between the constituent objects reflect functionality of the system. The objects are represented as nodes/vertices and the directional or mutual interactions/relations are represented by the directed or undirected edges between components. Social networks interactions [Qiu18], telecommunication interactions [Cor01], recommender systems [Wu19], molecular interactions in chemistry [Gil17], grammatical relations between words of a sentence [Mar17], etc. are some of the graphically represented systems.

Anomaly detection on graph data has been an active research area [Ako15]. Especially, graph-based anomaly detection finds its application in Cybersecurity for spam and malware detection [Cas07, Ben05] in Web network, socware (malware in social networks) detection in Social networks [Rah12], and cyber-attacks and intrusion detection in computer networks [Xia20, Ili11].

An industrial communication network can be represented as a graph, where industrial components and networking assets constitute nodes and the communication relationships between them are represented as edges of the graph. The communication relationship modeled on the edges represent the nature of the graph as static or dynamic. The connectivity information embedded in the graph are exploited for network optimization [Alm19], network planning [Zhu21] and deployment of network security countermeasures.

The process data communication relationships between industrial components could be modeled in a graph and used for process data analysis to detect anomalies in the industrial process. The network topology remains static however the values on the edges are dynamic. The structural information and
temporally changing edge information offers insights into spatio-temporal characteristics of industrial networks.

In this chapter, the challenge of representing the spatio-temporal characteristics of an industrial process as a Graph and self-learning the process behaviour for anomaly detection is addressed. The research problems concerning the representation and learning are formulated in section 5.1 followed with the foundational information on Graph Representation Learning in section 5.2. The proposed solutions for the representation and learning of an Graph-represented industrial process are described in section 5.3 - section 5.5. The chapter is reviewed and concluded in section 5.6.

5.1 Research Problem

Threat actors target the spatial and temporal characteristics (the periodic and deterministic requirements) of an industrial process through violating integrity and availability requirements of industrial communication [Rub17]. The threat behaviours in the traffic could be detected efficiently through Graph-based analysis only when the industrial network’s Graph representation aptly represents the spatio-temporal characteristics of its communication. After an appropriate spatio-temporal characteristics representation on a graph is available, a Machine Learning (ML) model can learn the normal process behaviours and detect the deviations as anomalies.

In a self-learning process behaviour analysis of industrial networks, the spatio-temporal characteristics are extracted from the industrial traffic and represented as a graph. A ML model learns the normal process behaviour from the normal operations of industrial process, and the model is utilized for anomaly detection in process data exchange. Graph Neural Networks (GNN) [Mer05, Sca08] are the ML models exclusively developed for graph data analysis. In recent years, GNN have gained attention for analysis of graph-structured data and have shown to perform better in graph classification, node classification,
5.1 Research Problem

edge classification and link prediction tasks [Zho20b]. Its applications in Cybersecurity for botnet detection [Zho20a], malware detection [Bus21] and network intrusion detection [Puj21] have been reported.

Figure 5.1: Graph representation of the Festo Demonstrator’s industrial network communication.

In the presented work, for a given PROFINET-based industrial system (the Festo Demonstrator, refer section 2.5), its process data exchange is represented as a graph, as shown in fig. 5.1. The edges represent Connections between industrial components and changing edge values represent process data exchange. A spatio-temporal graph representation is required to capture the spatio-temporal characteristics extracted from PROFINET traffic. Feasibility of GNN to model process behaviour based on the spatio-temporal graph representation for anomaly detection needs an evaluation. The research problem of self-learning the process behaviour in Graph represented data is formulated as follows:

1 How to model spatio-temporal characteristic of industrial communication in Graph representation? [Addressed in section 5.4]
2 How to learn Graph-represented process behaviour? \([Addressed\ in\ \text{section}\ 5.5]\)

3 How to classify Graph-represented process data as normal or anomalous? [Addressed in section 5.5]

### 5.2 Foundations

Formally, a graph \(G=(\mathcal{V}, \mathcal{E})\) defines set of nodes \(\mathcal{V}\) and interactions/relations between nodes as set of edges \(\mathcal{E}\). An edge \(e_{ij} \in \mathcal{E}\) is defined as directed/undirected link between nodes \(v_i\) and \(v_j\), \(v_i, v_j \in \mathcal{E}\). In case of directed relations, \(e_{ij} \neq e_{ji}\). The structural information of a graph or its topology is represented by an adjacency matrix \(\mathcal{A}\). Each element of the matrix \(a_{ij} \in \mathcal{A}\) represents the edge information between nodes \(v_i\) and \(v_j\) i.e. \(a_{ij} = 1\) if \(e_{ij} \in \mathcal{E}\), otherwise \(a_{ij} = 0\). If there are no self-loops on the nodes, the diagonal elements are 0, and for undirected graphs \(\mathcal{A}\) is diagonally symmetrical. A complete graph contains an unique edge between every pair of nodes. If the graph is not a complete graph, the \(\mathcal{A}\) is a sparse matrix and utilizing it for graph analysis task is computationally expensive. To circumvent the computational overload, the edge connectivity is represented as coordinate list (COO) of node indices tuples, such that tuple \((i, j)\) represents edge between nodes \(v_i\) and \(v_j\).

In homogeneous graphs, the nodes and edges have same types, whereas nodes and edges have different types in heterogeneous graphs. Social networks are homogeneous graphs where nodes are persons and edges represent relationship between them. In heterogeneous biomedical graphs, the nodes could be either proteins, drugs or diseases and edges between protein-drug and drug-disease represent different information such as inhibitor and treatment relations, respectively.

Any domain’s data represented as graphs are analysed with ML methods to extract problem-driven solutions to its underlying problem use cases. The foremost requirement for any ML pipeline is defining features that captures the information embedded in graph data. Node-level features of graphs are represented by matrix \(X \in \mathbb{R}^{\mid\mathcal{V}\mid \times m}\), where each node is represented
as $m$-dimensional real-valued vector. When edge-level features are available, the elements of adjacency matrix $\mathcal{A}$ are represented as $a_{ij} \in \mathbb{R}^k$ for $k$-dimensional real-valued vector.

The ML tasks in the context of graph analysis can be summarized as follows:

1. Node-level tasks either classify nodes into categories (node classification), predict real-value of nodes (node regression) or group similar nodes together (node clustering). In a citation graph, classification of node-represented documents to a topic is an example of node classification [Kip16].

2. Edge-level tasks aim to either classify edge types (edge classification) or predict a relation/link between nodes (link prediction). Predicting a drug’s side-effects in biomedical graphs is an example of link prediction [Zit18].

3. Graph-level tasks consist of predicting real-valued properties of a graph (graph regression), classify graphs into categories (graph classification) and grouping similar graphs together (graph clustering). Predicting toxicity of a molecule is an example of graph regression [Gil17]. For graph-level tasks, the node features (and edge features) are used in the model for analysis.

In a transductive learning setting, the ML model evaluates on nodes provided in training phase. For new unseen nodes, the training phase is performed again. In contrast, the models learnt in inductive setting evaluates new unseen nodes without the need of retraining.

The Traditional ML approaches on graphs utilize graph statistics and kernel methods for node and graph classification tasks. In particular, node degree, node centrality, clustering coefficient for node’s local neighbourhood are node-level features used for node classification tasks. For graph classification tasks, graph-level features are extracted through graph kernel methods.
such as bag of nodes, the Weisfeiler-Lehman kernel, graphlet (subgraph structures) kernel, path-based random walk and shortest-path kernels. The node-level and graph-level features used for classification tasks do not take the relationships between nodes into consideration. For edge prediction tasks, a new measure quantifying the neighbourhood overlap between nodes have been used. For the local overlap statistics, Sorensen index, Salton index, Resource Allocation index, etc. have been proposed. When two nodes do not share a local neighbourhood but belong to same community in the graph, global overlap statistics have been proposed for such use cases. Katz index, LHN similarity and random walk method such as PageRank approaches are path-based similarity measures developed for quantifying global neighbourhood relationships. For details on the mentioned graph statistics, refer to Chapter 2 of Hamilton’s *Graph Representation Learning* [Ham20].

The traditional ML approaches on graphs are limited due to hand-engineered statistics and measures which are inflexible to adapt to a learning process and expensive to design and implement. As an alternative to limiting hand-engineered feature extraction, the *graph representation learning* approach learns the representations embedded with structural information of a graph. As outlined in [Ham20], the graph representation learning is viewed as the framework of encoding and decoding graphs to learn low-dimensional vectors or *embeddings*. An encoder model encodes the graph’s positional and local neighbourhood structural information of nodes in low-dimensional vectors. The decoder model takes the node embeddings to reconstruct node neighbourhood and other graph statistics in the original graph.

Formally, for a pair of nodes \( u, v \in V \), an encoder function \( ENC \), a decoder function \( DEC \), a similarity measure between two nodes in a graph \( S, z_u, z_v \in \mathbb{R}^d \) as \( d \)-dimensional node embeddings, the encoder-decoder framework is summarized as follows:

\[
\begin{align*}
ENC : V & \rightarrow \mathbb{R}^d \\
DEC(ENC(u), ENC(v)) & = DEC(z_u, z_v) \approx S[u, v]
\end{align*}
\]

The reconstruction objective is to minimize the reconstruction loss \( \mathcal{L} \) over a set of node pairs \( \mathcal{D} \):
\[ L = \sum_{u,v \in D} l(DEC(z_u,z_v), S[u,v]) \]

where \( l \) is the reconstruction loss function, usually mean-squared error or cross entropy loss.

The **Shallow Embedding** approach defines the encoder function as a lookup of a node based on its ID in a node embedding matrix \( \mathbf{Z} \in \mathbb{R}^{|\mathcal{V}| \times d} \). The well known shallow embedding methods are motivated by matrix factorization and random walks. In matrix factorization, the decoder reconstructs the entries into the adjacency matrix of a graph from low-dimensional node embeddings with approximation on node-node similarity matrix \( S \). Graph Factorization approaches, GraRep and HOPE are examples of shallow node embedding algorithms using matrix factorization. DeepWalk, node2vec and large-scale information network embeddings are random walk based shallow node embedding algorithms. The node embeddings are optimized such that the two nodes co-occurring on short random walks over graph have similar embeddings. There are drawbacks to shallow embedding approaches: (a) no parameters are shared between nodes in the encoder, hence, the number of parameters grow linearly as number of nodes increases (computationally inefficient), (b) the node features are not utilized in the encoder, and (c) transductive learning setting i.e. doesn’t generalize to unseen nodes.

## 5.3 Graph Neural Networks

**Graph Neural Networks (GNN)** are a neural network framework for graph data with encoders defined over the graph structure and its attributes. The motivation of utilizing neural networks for graph data is found in the works of Bruna et al. [Bru13] to generalize convolutions to non-Euclidean data, Dai et al. [Dai16] defining a differentiable variant of belief propagation and Hamilton et al. [Ham17a] outlining graph isomorphism tests. At its core, a GNN employs a form of **neural message passing**, where for a given graph \( G=(\mathcal{V}, \mathcal{E}) \) and its node features \( \mathbf{X} \in \mathbb{R}^{|\mathcal{V}| \times d} \), the information as vector messages are exchanged between nodes and updated through neural networks to generate node embeddings \( z_u, \forall u \in \mathcal{V} \) [Gil17]. In message-passing iteration of GNN,
a hidden embedding $h_u$ for each node $u \in V$ is updated with information aggregated from $u$’s graph neighbourhood $\mathcal{N}(u)$, as shown in fig. 5.2. In fig. 5.2, the message-passing computations of GNN over the graph for its full neighbourhood is shown on the right.

Figure 5.2: The demonstration of GNN computation [Ham17b].

The message-passing update process [Ham20] can be summarized as:

$$h_u^{(k+1)} = UPDATE^{(k)}(h_u^{(k)}, AGGREGATE^{(k)}(\{h_v^{(k)} \forall v \in \mathcal{N}(u)\}))$$

(5.3)

where, $UPDATE$ and $AGGREGATE$ are differentiable functions and $m_{\mathcal{N}(u)}$ is the “message” containing aggregated information from node $u$’s graph neighbourhood $\mathcal{N}(u)$. The superscripts represent embeddings and functions at different iterations of message passing, or different layers of GNN.

### 5.3.1 Basic Intuition

At each iteration/layer $k$ of GNN, every node aggregates embeddings of its local neighbouring nodes in the graph and updates its own embeddings. As the iterations progresses, the information of the further reaches in the graph are aggregated into node’s embeddings. The initial embedding for a node $u$ is its
input features i.e. at \( k = 0, h^{(1)}_u = x_u, \forall u \in V \). At \( k = 1 \), node \( u \)'s 1-hop neighbourhood is aggregated in \( h^{(1)}_u \) i.e. all the nodes that are immediate neighbours with graph path length 1. At \( k = 2 \), \( h^{(2)}_u \) contains 2-hop neighbourhood information, and so on. After \( K \) iterations of message-passing and updates, the final layer outputs the embeddings of each node, \( z_u = h^{(K)}_u, \forall u \in V \). It summarizes structural information such as node degrees and feature-based information of nodes in its \( K \)-hop neighbourhood. The local neighbourhood information aggregation is analogous to convolutional operation in Convolutional Neural Network, where feature information is aggregated over local graph neighbourhood instead of spatially-defined patches in an image [Dai21].

### 5.3.2 Basic GNN

The abstract definition of message-passing in a GNN described so far can be translated to a general instantiations in two classes as follows:

(a) **isotropic GNN**, where every neighbouring edge is treated equally in the update equation:

\[
    h^{(k)}_u = \sigma(W_{self} h^{(k-1)}_u + W_{neigh} \sum_{v \in N(u)} h^{(k-1)}_v)
\]

(b) **anisotropic GNN**, where every neighbouring edge is weighted different:

\[
    h^{(k)}_u = \sigma(W_{self} h^{(k-1)}_u + W_{neigh} \sum_{v \in N(u)} \eta_{uv} h^{(k-1)}_v)
\]

\[
    \eta_{uv} = f^{(k-1)}(h^{(k-1)}_u, h^{(k-1)}_v)
\]

where \( W_{self}, W_{neigh} \in \mathbb{R}^{d^{(k)} \times d^{(k-1)}} \) are trainable parameter matrices, \( \sigma \) is a non-linear element-wise activation such as ReLU or \( \text{tanh} \), and \( f \) is a parametrized function on edge between nodes \( u \) and \( v \).

Different GNN instantiations of isotropic and anisotropic GNN, which are evaluated for process data analysis, are outlined in section 5.5.
5.3.3 Graph Pooling

After \(K\)-iterations, the node embeddings \(z_u, \forall u \in V\), for a graph are computed. However, in a graph-level task, an embedding over the graph \(G, z_G\) is required. The graph embedding can be learnt through pooling the node embeddings over final GNN layer together to calculate their sum (or mean) \([Ham20]\):

\[
z_G = \frac{\sum_{u \in V} z_u}{f_n(|V|)},
\]

where \(f_n\) is the normalizing function.

5.4 Spatio-temporal Graph Representation

In order to capture the spatio-temporal characteristics of an industrial system’s network communication, Payload Bytes Profiling (PBP) framework’s sequential steps from Payload Byte Extraction to Transition Interval Computation are employed, as shown in fig. 5.3.

![Figure 5.3: The Payload Byte Encoding steps from PBP.](image-url)
The transition order of the alphabet-encoded process payload bytes corresponds to the spatial characteristics and the transition interval represents the temporal characteristics. In the current case of graph representation of industrial network communication, we encode the spatio-temporal characteristics of process data exchange over the edges of Connection between industrial components (IOController, IODEvice), as shown in fig. 5.4. Additionally, the network transmission characteristics are added as the Cycle Counter value differences between transitioning process payload bytes. The cycle counter value in a PNIO frame serves the purpose of up-to-dateness determination of frame and detect duplicate frames. Based on the deterministic time interval in process data transmission, the cycle counter values are incremented in fixed iterations and reset after the cycle is complete. The difference in cycle counter values of transition process payload bytes encapsulates either transition from higher counter valued frames to lower counter frames (-ve) or vice-versa (+ve). In a nutshell, as shown in fig. 5.4, the edge features of the Connection between components is defined as tuple (previous payload byte, current payload byte, transition interval, cycle counter difference).

Figure 5.4: Spatio-temporal industrial network characteristics modeling on Graph.
In order to represent the spatio-temporal characteristics of the process, a graph snapshot is defined on a fixed time window over the traffic, shown in fig. 5.5. The graph snapshot contains the homogeneous graph representation of the industrial system’s network communication, where features of each Connection edge are updated as per transition information of the window. The window size is defined as number of Output Connections of the industrial network.

Significance of encoding: Within the graph snapshot, the correlation of process payload bytes between Connections are encoded. It encodes following implicit information:

1 the relation between the current payloads of all Connections, and
2 the relation between intra-Connection transitions, along with their temporal transition intervals.

Especially, when the transition of payload bytes in one of the Connection remains persistent for long time, its effect on the behaviour of other Connections can be easily captured. In theory, stealthy attacks on industrial processes
through manipulation of Cycle Counters in PROFINET traffic outlined by Ferrari et al. [Fer20] can be detected. The cycle counter differences encoded over the edge will have inconsistent values compared to normal behaviour.

**Binary Encoding.** For representing numerically the encoded process payload byte and devices, one-hot encoding is incorporated. For encoding the values of intervals and counter differences, each float value is 32-bit encoded. For example, A1 and B1 alphabet-encoded transitioning payload bytes for Connection PLC-2~BK-2 are one-hot encoded over the edges, as shown in fig. 5.6. The interval values 32.0 seconds and counter differences 2600 are binary encoded. The edge feature for every Connection in the graph snapshot has length 76 (6 + 6 + 32 + 32), and node feature size is 8.

![Binary Encoding of node and edge features.](image-url)
5.5 Graph-based Process Data Analysis

The industrial network communication characteristics are represented as *Graphs*, where edges represent logical network connection between industrial components for process data exchange. GNN are the ML models being employed to learn the characteristics. They learn the structural information of logical network topologies and process exchange traffic characteristics encoded over the edges in edge features, as outlined before. The ML task for GNN is to classify *graph snapshots* for *normal* or *abnormal* industrial process behaviour (*graph classification*). Different GNN architectures are evaluated for their performances on learning the normal behaviour, and capability to distinguish anomalies triggered by process data targeted ‘Force Attack’ (refer fig. 2.13).

5.5.1 GNN Variants

There have been multiple GNN variants developed in recent years varying in their UPDATE and AGGREGATE functions. In this work, *Graph Convolutional Network* (GCN) for an isotropic GNN, and *Message Passing Neural Network* (MPNN), *Gated Graph ConvNet* (GatedGCN) and *Graph Transformer* (GT) anisotropic models have been employed for proposed solution. The selection of anisotropic models is driven by their usage of edge attributes for GNN computation and implementation availability amongst the published GNN architectures.

(a) Graph Convolutional Network (GCN) is the baseline GNN model, outlined by Kipf et al. [Kip16], that employs symmetric normalization for isotropic aggregation of neighbourhood information of a node along with its own information.

\[
h_u^{(k+1)} = \text{ReLU}\left( W^{(k)} \sum_{v \in \mathcal{N}(u) \cup \{u\}} \frac{h_v^{(k)}}{\sqrt{|\mathcal{N}(u)||\mathcal{N}(v)|}} \right),
\]
where $W$ is the learnable parameter matrix, $h_u, h_v \in \mathbb{R}^d$ are node embeddings and $\mathcal{N}(u)$ is the neighbourhood of node $u$.

(b) Message Passing Neural Network (MPNN) is a GNN framework, outlined by Gilmer et al. [Gil17], that operates on node features $x_u, u \in \mathcal{V}$ and edge features $e_{uv}, e_{uv} \in \mathcal{E}$ of a given graph to generate node embeddings.

$$h_u^{(k+1)} = \text{ReLU}(W^{(k)}h_u^{(k)} + \sum_{v \in \mathcal{N}(u)} h_v^{(k)}h_\mathcal{E}(e_{uv})),$$

where, $h_\mathcal{E}$ is a multilayer perceptron to embed edge features, $W$ is the learnable parameter matrix, and $h_u, h_v \in \mathbb{R}^d$ are node embeddings.

(c) Graph Transformer (GT) outlined in Shi et al. [Shi20] adopts multi-head attention mechanism from Transformer architecture of Vaswani et al. [Vas17], with inclusion of edge features for graph learning. An “attention” defines the weight of an edge in a node’s neighbourhood as per its influence in aggregation computation.

$$h_u^{(k+1)} = \text{ReLU}(W_1^{(k)}h_u^{(k)} + \sum_{v \in \mathcal{N}(u)} \alpha_{uv}(W_2^{(k)}h_v^{(k)} + W_6^{(k)}e_{uv}))$$

$$\alpha_{uv} = \text{softmax} \left( \frac{(W_3^{(k)}h_u^{(k)})(W_4^{(k)}h_v^{(k)} + W_6^{(k)}e_{uv})}{\sqrt{d}} \right),$$

where, $W_1, W_2, W_3, W_4, W_5$ and $W_6$ are the learnable parameter matrices, $e_{uv}$ is the edge feature, $\alpha_{uv}$ is the attention-coefficient for edge $e_{uv}$, and $d$ is the size of head.

(d) Gated Graph ConvNet (GatedGCN) is the GNN architecture proposed by Bresson et al. [Bre17] leveraging the vanilla graph ConvNet architecture of Sukhbaatar et al. [Suk16] and the edge gating mechanism of Marcheggiani et al. [Mar17]. Unlike other anisotropic GNN models, GatedGCN explicitly update edge features along with node features at each iteration:

$$h_u^{(k+1)} = \text{ReLU}(W_1^{(k)}h_u^{(k)} + \sum_{v \in \mathcal{N}(u)} \eta_{uv} \odot W_2^{(k)}h_v^{(k)}),$$
where, $W_1$ and $W_2$ are learnable parameter matrices, $h_u, h_v$ are node embeddings, $\odot$ is Hadamard product, and $\eta_{uv}$ are the edge gates computed as:

$$\eta_{uv} = \frac{\sigma(e_{uv}^{(k)})}{\sum_{v \in N(u)} \sigma(e_{uv}^{(k)}) + \epsilon}$$

$$e_{uv}^{(k)} = \text{ReLU}(A^{(k)} h_u^{(k-1)} + B^{(k)} h_v^{(k-1)} + C^{(k)} e_{uv}^{(k-1)})$$

where, $\sigma$ is the sigmoid function, $e_{uv}$ are edge features, $\epsilon$ is the fixed constant for numerical stability, and $A, B$ and $C$ are learnable parameter matrices.

### 5.5.2 Dataset

**Negative Sampling.** The spatio-temporal modeling of network traffic contains only the normal behaviour of industrial network communication. For a ML model to self-learn the normality in absence of any known abnormality, the data with abnormal characteristics are generated artificially. They can be generated in multiple ways for a given domain, which is the case for current work. The following amongst the many other ways are chosen to generate abnormal characteristics data in the presented study: (1) abnormal transition order of payload bytes for inter-Connection transitions, (2) abnormal transition intervals outside the observed interval ranges of normal transitions, and (3) abnormal cycle counter differences outside the observed ranges of normal transitions.

**Training Dataset.** The training dataset consists of graph snapshots extracted over data captured from normal behaviour, refer section 2.5.4. Every graph snapshot is a graph consisting of 8 nodes and 7 edges with feature size 8 for a node and 76 for an edge. The negative sampled data was added to weigh in abnormalities as per the selected methodologies in section 5.5.2. The dataset was split into 80:20 ratio for train and validation for training of GNN models:

- Training Dataset: 1139 normal snapshots, 261 negative-sampled abnormal snapshots
5.5 Graph-based Process Data Analysis

- Validation Dataset: 489 normal snapshots, 113 negative-sampled abnormal snapshots

**Test Dataset.** To evaluate the anomaly detection performance, the traffic captured while executing network attacks is used for extracting snapshots. The anomaly use case is outlined in fig. 5.7. The process parameters on the output data exchange for Connection PLC-2-BK-2 are modified, which causes Lower Belt to move in reverse direction. The faulty process payload byte transition is encoded over the edge between PLC-2 and BK-2 of the graph snapshot. All the graph snapshots containing the faulty payload byte transition are considered abnormal, otherwise normal. The test dataset contains 41 normal snapshots and 47 abnormal/anomalous snapshots. Every graph snapshot is a graph consisting of 8 nodes and 7 edges with feature size 8 for a node and 76 for an edge.

![Graph snapshot diagram](image)

**Figure 5.7:** The anomaly use case of modifying parameter.

### 5.5.3 Analysis Pipeline

Dwivedi et al. [Dwi20] outlined an experimental pipeline for benchmarking of GNN, shown in fig. 5.8, and it has been incorporated in this work. The graph and its features are given as input to the **Input Layer**, followed by convolutional computations in **GNN Layer** and graph classification task in the **Prediction Layer**.
Input Layer. The node features \( \alpha_i \in \mathbb{R}^{a \times 1} \) for every node \( i \) and edge features \( \beta_{ij} \in \mathbb{R}^{b \times 1} \) for every edge between nodes \( i \) and \( j \) are linearly projected to \( d \)-dimensional hidden features \( h_i^{l=0} \) and \( e_{ij}^{l=0} \), respectively:

\[
    h_i^0 = W_1^0 \alpha_i; \quad e_{ij}^0 = W_2^0 \beta_{ij}
\]

where \( W_1^0 \in \mathbb{R}^{d \times a} \), \( W_2 \in \mathbb{R}^{d \times b} \).

GNN Layer. Each GNN Layer computes hidden features for each node and edge of the graph through recursive message passing in the local neighbourhood of each node. \( L \) GNN layers are stacked for \( L \)-hop neighbourhood message passing computations. For the graph snapshots, \( L \) is defined by the depth of graph snapshot to allow message diffusion throughout the network. In the
presented work and the industrial system under consideration, we employ 2 GNN layers for 2-hop neighbourhood computation, refer fig. 5.9.

**Prediction Layer.** We pool final node embeddings of all the nodes to embed the graph’s features, refer section 5.3.3. A Multi-Layer Perceptron (MLP) is employed over the graph embeddings $z_G$ for the graph classification task.

### 5.5.4 Implementation Frameworks

The analysis pipeline was realized in Python utilizing PyTorch Geometric (PyG) [Fey19] and Deep Graph Library (DGL) [Wan19] libraries for GNN architecture layers. Particularly, PyG implementations of GCN, MPNN, GT and DGL implementation for GatedGCN are utilized. Both the libraries require their own representation of datasets, hence, train and test snapshot datasets were converted into respective library formats. In addition, the libraries work over the batches of dataset for training and evaluation of GNN models.

In order to regularize the model parameters over different batches of dataset, batch normalization (BN) is augmented to each GNN layer. For every iteration of message passing,

$$h_u^{(k+1)} = UPDATE^{(k)}(BN(h_u^{(k)}, AGGREGATE^{(k)}([h_v^{(k)}, \forall v \in \mathcal{N}(u)]))$$

where, UPDATE and AGGREGATE are differentiable functions, $\mathcal{N}(u)$ is node $u$’s graph neighbourhood and $h_u, h_v$ are node embeddings.

**Binary Cross Entropy** (BCE) is utilized as the loss function to train GNN models for the graph classification task, which is defined as:

$$BCE = -t_1 \log(\sigma(s_1)) - (1 - t_1) \log(1 - \sigma(s_1))$$

where, $t_1$ and $s_1$ are ground truth and classification score of the sample for class $C_1$ of binary classes $\{C_1, C_2\}$, and $\sigma$ is the sigmoid function.

**Performance Metrics.** Specificity is used to measure the GNN model’s performance on detecting anomalies, whereas Sensitivity measures recall performance on normal graph snapshots, refer section 4.4.2.
System Configuration. The GNN models are computed in the Colab Pro environment with a Tesla P100-PCIE-16GB GPU offered by Google Research¹.

5.5.5 Hyperparameter Optimization

The parameters of the learning process and model parameters for different configurations of every GNN architecture are evaluated with the Training Dataset, to get the best model settings for each GNN architecture. The table 5.1 summarizes all the parameters which were optimized to get the best model configurations for each GNN architecture. For different configuration instances of each GNN architecture, the one with best performance on the Validation Dataset with high Sensitivity measure is chosen as the best model of the GNN architecture.

The number of epochs is the number of times the training dataset is passed forward and backward through the GNN. When the epochs are very low, the model is underfitting as the GNN has not learnt enough. On the other hand, the model might overfit the learning for too high epochs. The batch size defines the number of sub-samples from training data as input to the GNN before the weights are updated. A bigger batch size slows the learning process, whereas the lower batch size fastens the learning process. The learning rate controls the frequency of updating the weights at the end of each batch. A very small learning rate results in slow converging of the model, and the too large learning rate would diverge the model.

Table 5.1: Summary of hyperparameter optimization of GNN models.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value Options</th>
<th>GCN</th>
<th>MPNN</th>
<th>GT</th>
<th>GatedGCN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Epochs</td>
<td>[300]</td>
<td>60</td>
<td>200</td>
<td>100</td>
<td>150</td>
</tr>
<tr>
<td>Batch Size</td>
<td>[16, 32, 64]</td>
<td>16</td>
<td>32</td>
<td>16</td>
<td>32</td>
</tr>
<tr>
<td>Learning Rate</td>
<td>[0.1, 0.01, 0.001, 0.0001]</td>
<td>0.1</td>
<td>0.01</td>
<td>0.001</td>
<td>0.001</td>
</tr>
</tbody>
</table>

¹ https://colab.research.google.com/
5.5.6 Evaluation Performance

The GNN architecture models with optimized parameter are evaluated on the Test Dataset, for their performances on detecting anomalies and recalling the learnt normal behaviour of the industrial process. The dataset contains 41 normal snapshots and 47 abnormal/anomalous snapshots, refer section 5.5.2. The anomalous snapshots contains the faulty process payload byte transition encoded over the edge between PLC-2 and BK-2. The time taken for each hyperparameter-optimized GNN architecture with number of model parameters are summarized in table 5.3. The performance of GNN architectures for anomaly detection are summarized in table 5.2.

Table 5.2: Comparison of different GNN architectures’ performance on anomaly detection and spatio-temporal modeling.

<table>
<thead>
<tr>
<th>GNN Model</th>
<th>Specificity</th>
<th>Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>GCN (Baseline)</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>MPNN</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>GT</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>GatedGCN</td>
<td>1.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>

The isotropic GCN model couldn’t distinguish between normal and anomalous graph snapshots as the information is encoded on the edge features. Since, the network structure remains constant in either evaluation case and is similar to learnt normal behavioural graph structure, GCN recalls all the normal graph snapshots successfully.

The anisotropic GNN models detected the anomalies completely with complete recall on normal graph snapshots. For the proposed spatio-temporal characteristics encoding on the edges (refer section 5.4), the anisotropic GNN models could be incorporated for anomaly detection. The information on the edges of different connections could be enriched for analysis in more complex use cases than 'Force Attack', such as Stealthy Attack outlined in the work of Ferrari et al. [Fer20].
The evaluation result concludes the correctness of encoding mechanism outlined in section 5.4 for modeling spatio-temporal graph representation. The Sensitivity score indicates that the anisotropic GNN are able to learn process behaviour of the industrial network based on the spatio-temporal encodings on the edges. The Specificity score conveys the applicability of Graph pooling for the graph classification task as process data anomaly detection method. The detection of ‘Force Attack’ by the anisotropic GNN based on the spatio-temporal encodings on the edges satisfies the BSI’s “Category D - unusual changes in process data” requirement to detect anomalies in an industrial process, as outlined in section 1.1.1.

Table 5.3: Execution time of GNN architectures.

<table>
<thead>
<tr>
<th>GNN Model</th>
<th>Model Parameter Count</th>
<th>Computation Time per 10 Epoch (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GCN (Baseline)</td>
<td>3,201</td>
<td>7.6</td>
</tr>
<tr>
<td>MPNN</td>
<td>75,361</td>
<td>4.2</td>
</tr>
<tr>
<td>GT</td>
<td>29,089</td>
<td>11.0</td>
</tr>
<tr>
<td>GatedGCN</td>
<td>187,521</td>
<td>6.9</td>
</tr>
</tbody>
</table>

The time taken to execute GNN architectures are low as the size of every evaluated graph snapshot, normal and anomalous, is small - 8 nodes and 7 edges. For a large industrial system, when the process complexity increases, the number of nodes and edges of the networking graph increases. The larger the size of graph, more the number of model parameters. Consequently, the GNN computation time would grow.

5.6 Discussion and Summary

5.6.1 Review

In the recent years, analogous to presented work, applications of GNN for network cybersecurity based on features extracted from network traffic have been published.
Zhou et al. [Zho20a] incorporated GCN for botnet detection. A synthetic botnet topology is overlayed on a large-scale real networks and topological information is extracted from network traffic flows. The graph representation of the network does not contain any flow features on the edges or nodes of the graph. Based solely on the connectivity information, GCN classifies nodes as part of botnet or normal infrastructure (node classification task).

Pujol-Perich et al. [Puj21] presented GNN’s potential as robust intrusion detection methodology. The network flows between network assets are represented as a heterogeneous host-connection graph to model the structural relationships between different network flows. The host nodes represent the network assets, flows between assets are represented by the connection nodes and the directed edges connect the flows to source and target hosts. A GNN model based on the heterogeneous graph representation with Gated Recurrent Units [Chu14] as UPDATE functions (refer eq. (5.3)) for embedding flow relationships is proposed. The embeddings of connection nodes are classified for specific attacks (DDoS, port scan or network scans) or benign traffic (node classification task).

The usage of Spatio-Temporal Graph Convolutional Network (STGCN) [Yu17] for Distributed Denial-of-Service (DDoS) attack detection is outlined in the work of Xie et al. [Xie20]. The network flow features extracted from windows over the traffic are utilized to represent characteristics of all the nodes in the topology graph of the monitored network: total source packets, total source bytes, total destination packets, total destination bytes and unknown TCP traffic. STGCN is shown to effectively correlate spatio and temporal features between network nodes for the underlying node classification task of DDoS attack detection.

GCN SCOPE [Oba20] is a graph convolutional network-based suspicious communication pair estimation framework, which learns the embeddings of IP addresses of a network from its communication triplets using relational graph convolutional networks (R-GCNs) [Sch18]. It quantifies anomalous unobserved communication triplets, each triplet is a tuple of server IP address,
TCP/UDP port and client IP address. A multigraph is constructed from communication triplets, and R-GCN is used for link prediction task to score unobserved communication triplet.

E-GraphSAGE [Lo21] is a GNN-based intrusion detection system inspired from GraphSAGE algorithm [Ham17b] to capture edge features in addition to topological information and node features. The network flow features are represented over the edges of graph representing network communication for graph representation learning. E-GraphSAGE samples its neighbouring nodes and corresponding edges of all the nodes to compute node and edge embeddings. The edge embeddings are used for edge classification task of network flow classification.

NF-GNN [Bus21] is a network flow graph-based approach for traffic-based malware detection. A network flow graph extracted from traffic consists of nodes corresponding to network endpoints and edges represent the network flow features of connection between endpoints. A GNN model tailored for network flow graph representation is proposed to compute graph embeddings for supervised/unsupervised graph classification task of malware detection.

The presented work in this chapter differs from the published literature in terms of graph representation of network traffic and the ML task. The industrial network communication is represented through directed homogeneous graph (refer section 5.4), which differs from the work of GCN SCOPE and Pujol-Perich et al. E-GraphSAGE samples the neighbourhood information, whereas complete neighbourhood information is required for process data analysis (refer section 5.5). The task of NF-GNN is similar to this chapter’s proposed solution of utilizing GNN for process data analysis in industrial networks, hence, its usage for evaluation is scheduled as component of future work.

5.6.2 Conclusion

In this chapter, different Graph Neural Networks (GNN) architectures are evaluated for modeling spatio-temporal characteristics of PROFINET networks.
to detect process data anomalies. A graph representation to encode the *spatio-temporal* characteristics on the edges is presented. *Isotropic* Graph Convolutional Network (GCN) and *anisotropic* Message Passing Neural Network (MPNN), Graph Transformer (GT) and Gated Graph Convolutional Network (GatedGCN) instances are utilized to learn process behaviour from the normal operations of industrial process. Negative sampling is utilized for the learning process. The anomaly use case of ‘Force Attack’ on the *Festo Demonstrator* is employed for anomaly detection performance evaluation. Graph pooling for the graph classification task is defined as the anomaly detection methodology. The evaluation results show that GNN are capable to learn *spatio-temporal* characteristics of process data exchange in industrial networks for anomaly detection. Thus satisfying the BSI’s “Category D - unusual changes in process data” requirement to detect anomalies in an industrial process, as outlined in section 1.1.1.

In comparison to published GNN literature for Cybersecurity, NF-GNN [Bus21] is the closest fit as additional GNN architecture to be considered in future evaluations compared to E-GraphSAGE [Lo21], GCN SCOPE [Oba20] and GNN architecture of Pujol-Perich et al. [Puj21]. The size of an industrial system’s network and the complexity of its industrial process affects the size of node and edge feature encoding, consequently affecting the execution of the chosen GNN architecture computations. In conclusion, for an industrial system with deterministic industrial process, the process behaviour can be modeled as Graph with *spatio-temporal* characteristics encoded on the edges from its network traffic in a *self-learning* environment.
6 Conclusion

With the advent of 21st Century, the fourth industrial revolution interconnected physical industrial components with networking technology advancements to reduce production cost through efficient process control systems in the industrial production. The introduction of Ethernet-based protocols blurred the distinction between the IT office/enterprise networks and the OT ICS/industrial networks. The sensor in the production floor of an industrial production is made accessible to the personnel in the office/enterprise network. The traditional notion of Security by Obscurity to protect OT network from adversaries have been challenged by the cyber threats targeted at industrial systems in the last few decades (ref. table 1.2). The cybersecurity of industrial networks has become paramount with the adoption of new layered security design Security in Depth. Network-based intrusion detection system (NIDS) are one of the key countermeasure component in the layered security concept to detect cyber threats through monitoring the network traffic of an industrial communication network. The anomaly-based methods are effective in detecting unknown cyber threats in comparison to the signature-based methods for NIDS in industrial networks. Germany’s Federal Office for Information Security (BSI) in its cybersecurity recommendations on production networks [BSI19] outlined anomalies in industrial networks and related categories of feature requirements for the passively monitoring anomaly detection system (refer section 1.1.1). The anomaly detection system learns the industrial communication network’s topology, the communication links, time-related behaviour and communication content from the monitored network infrastructure information to flag the deviations as anomalies.
6 Conclusion

6.1 The Quest

When the access to the network infrastructure information of an industrial production is unavailable, configuring the NIDS for anomaly detection is challenging. An empirical solution is to self-learn the network infrastructure information (topology, assets and communication links) and the spatio-temporal behaviour from passive monitoring of industrial network traffic, in conjunction with anomaly detection systems to detect anomalies. However, in the absence of industrial process information, learning the process behaviour from the network traffic for anomaly detection is a challenge. Thus, the quest to find solutions for the research questions emerging from the challenge of self-learning anomaly detection in industrial production ensued the dissertation.

A self-learning framework for passive network monitoring and anomaly detection in industrial networks consisting of different analytical components is conceptualized as the structural skeleton to systematically explore the solutions for the research questions (ref. section 1.2). These analytical components are (a) data collection and network information extraction; (b) network information representation; and (c) network information analysis.

On the quest, the industrial system employed to develop and evaluate the solutions is the PROFINET-based Festo Demonstrator built at the IT-SECURITY LABORATORY, FRAUNHOFER IOSB (ref. section 2.5). It is a miniaturized manufacturing process mimicking a simplified painting closed-loop process scenario with PROFINET protocol for communication between real hardware components such as controllers and devices. In addition, two network-based cyber threats were executed during the process operations and the network traffic is passively captured from the network switch for the evaluation.

The contributions of the dissertation transpiring from the reported solutions for the research objectives and future prospects to better the results or resolve open questions are outlined in this chapter.
6.2 Industrial Network Transparency

Research Question 1: How to extract information of an industrial system from its network traffic?

Contributions. A Python-based systematic framework is conceptualized and developed to passively capture the network traffic from the PROFINET-based industrial system and extract the relevant network information to make the industrial network transparent for analysis. It dissects the network packets using Scapy framework to detect different networking operations of the industrial system. These networking operations reflect the multiple industrial operations an industrial system undergoes from start-up to the process data exchange. The network information that makes the industrial system transparent are network topology, assets and their attributes, communication links established between master and slave (referred as PROFINET Connection), time-stamped process data payload bytes. Thus satisfying the BSI’s “Category A - general requirements” for network transparency.

Discussion. The framework is modular to adapt different output information formats. However, the extracted network information that are relevant for further downstream data analyses are fixed. It contains the network topology, the process communication data and assets information for topology analysis, process data analysis and asset inventory, respectively. Additionally, the framework is not restricted to one industrial protocol either. To extract the information from another industrial communication protocol such as EtherNet/IP, the corresponding network packet dissector library need to be employed or developed when not available.

Outlook. The captured data is analysed offline in a batch process and the memory requirement is quadratic to the size of captured packets (PCAP). An online memory-efficient packet capture and simultaneous near to real-time information extraction module with parallelization capability is the next logical enhancement step. An open question with the research objective is, how to standardize the network information format to maximize its compatibility for open source analysis frameworks such as Security Onion [22c], Malcolm [22b].
6 Conclusion

6.3 Industrial Operations Behaviour

Research Question 2: How to enumerate and track an industrial system’s operations from network traffic?

Contributions. Finite State Machine (FSM) models are conceptualized and developed to represent the industrial operations and their transitions for devices, connections between master and slaves, and the industrial system. These FSMs model the valid industrial operations interpreted from PROFINET protocol specifications to detect different operation stages from the extracted network information and flag the invalid transitions as anomalies (ref. section 3.4). A Python-based framework PROFINET Operations Enumeration and Tracking (POET) is developed to realize FSMs and instantiate FSM Device, FSM Connection and FSM System for PROFINET devices, connections and the industrial system detected in the extracted network information (ref. section 3.4.4). POET successfully detected the implemented PN-DCP based network attack on the Festo Demonstrator mimicking an adversarial action to change the parameters of a configured PROFINET device during the process data exchange operation (ref. section 3.5.1). Consequently, POET satisfies the BSI’s “Category B - unusual or exceptional activities in an ICS network” requirements for detecting the change in protocol communication activity.

Discussion. POET is the first-of-its-kind Protocol-analysis based NIDS for PROFINET to incorporate empirical behaviour of PROFINET system collected from real-world systems. The conceptualized FSM models at the device-, connection- and system-level granularity can be applied to other Industrial Ethernet protocol based on its specification. Consequently, the stages and the transitions between the stages of industrial operations could be enumerated and tracked from the extracted network information. The industrial system’s operation behaviour could be learnt through FSMs and anomalies are detected as the invalid operations.

Outlook. Integrating POET to an event-based IDS such as Snort would trigger alarms when unwarranted protocol-based events are detected in the network traffic. The current version of POET uses empirical information collected from
Siemens PLC, however, the information could vary with other PLC environments such as CODESYS. Evaluating POET’s performance in CODESYS environment is the future work for robustness testing. Additional network attacks violating the valid industrial operations at all the granularities are needed to evaluate the anomaly detection performance of POET.

6.4 Spatio-temporal Process Behaviour

Research Question 3: How to represent the spatio-temporal characteristics of an industrial system’s process?

Contributions. In the absence of information on the programmed industrial process, there are no insights into the semantics of process values being exchanged. The spatio-temporal characteristics of the finite set of process payload bytes extracted from the process data frames are the representative of the embedded process values. The industrial process is conceptualized as the constituent of multiple sub-processes. Each sub-process represents the process data communication link established between a pair of master and slave devices exchanging a particular process parameter of the overall process.

In chapter 4, the String representation of ordered payload bytes where each process payload byte is alphabet-encoded has been outlined. The temporal information associated with payload bytes is utilized to define the transition intervals between pairs of adjacent encoded payload bytes, thus, capturing the spatio-temporal characteristics. A Python-based systematic framework Payload Bytes Profiling (PBP) has been developed to alphabet-encode the extracted process payload bytes and represent the spatio-temporal characteristics of an industrial system’s process and its constituent sub-processes into spatial (transition profile) and temporal (interval profile) profiles from passively monitored network traffic (ref. section 4.2.3).

In chapter 5, the ubiquitous Graph representation of an industrial network is additionally explored. The graph snapshot representation to capture the spatio-temporal characteristics of industrial process has been conceptualized and developed with nodes representing the industrial components and the
edges being the communication link between the components. The graph snapshot is created from the alphabet-encoded industrial process traffic and the transition interval information in conjunction with transitioning payload bytes and the differences in their Cycle Counter values are encoded on the edges over a fixed time window on the traffic (ref. section 5.4).

**Discussion.** The encoding of process data exchange as either String or Graph representation is applicable to any discrete and deterministic industrial process of an industrial production. The encoding scheme is also non-restrictive as the sequential order and the transition interval between the encoded payload bytes can be easily extracted with the knowledge of encoding scheme.

**Outlook.** The graph snapshot representation flattens out the temporal information over the edges. Another graph representation such as discrete temporal graphs with static nodes and evolving edges [Ska21] or spatial–temporal graph [Yu17] could be used to represent the spatio-temporal characteristics of an industrial process. In addition, the survey from Kazemi et al. [Kaz20] comprehends the representation learning for dynamic graphs which can act as preliminary reference to explore dynamic graph representations. Representation of the spatio-temporal characteristics of an industrial process as bitmaps/images is an interesting future work to lean on the advancements in Image Processing.

**Research Question 4:** How to learn the spatio-temporal characteristics of an industrial system’s process for anomaly detection from the network traffic?

**Contributions.** With two different conceptualized representations of industrial process traffic capturing its spatio-temporal characteristics, the process behaviour is learnt to distinguish anomalous behaviour from the normal.

In chapter 4, the Regular Expression-coupled Suffix Tree algorithm is conceptualized and developed to extract the transition profiles at the process and sub-process granularities from the alphabet-encoded process traffic. The transition profile for the process and its constituent sub-processes captures the periodically recurring alphabet-encoded process payload bytes sequence, thus, modeling the spatial characteristics of an industrial process/sub-processes (ref. section 4.3). For temporal characteristics modeling, the transition intervals between the transitions of process payload bytes in the transition profile of the
process/sub-process are modeled through non-parametric Machine Learning models Local Outlier Factor (LOF), Isolation Forest (IF) and One-Class Support Vector Machines (OC-SVM), and represents the temporal characteristics as the interval profile in PBP of a sub-process or the overall process, (ref. section 4.4). The PBP for Festo Demonstrator’s painting process is evaluated for anomaly detection performance when the network-based attack, ‘Force Attack’ (ref. section 2.5.3), changes the process values in a sub-process to move the Lower Belt component in the opposite direction. The anomalies triggered by the attack are successfully reported utilizing the transition profile of the sub-process PLC-2-BK-2 (ref. section 2.5.3).

In order to learn the spatio-temporal characteristics of an industrial process represented in graph snapshots, the anisotropic Graph Neural Network (GNN) architectures (Message Passing Neural Network (MPNN), Gated Graph Convolutional Network (GatedGCN) and Graph Transformer (GT)) are employed and evaluated for anomaly detection in chapter 5. The anisotropic GNN architectures learns the process behaviour with graph classification as the Machine Learning task to classify graph snapshots as normal or anomalous (ref. section 5.5). The anomalies triggered by the ‘Force Attack’ are successfully detected by the anisotropic GNN architectures, but the isotropic Graph Convolutional Network (GCN) model failed. It demonstrated the capability of anisotropic GNN architectures to utilize the edge features encoding the spatio-temporal characteristics in their learning.

As the PBP framework and anisotropic GNN architectures successfully detect the change in process values of an industrial process, they satisfy the BSI’s “Category D - unusual changes in process data” requirement of process-based anomaly detection.

Discussion. The PBP framework can be used for production cycle detection of an industrial process as demonstrated in section 4.6.1. To utilize the PBP framework in another Industrial Ethernet protocol based discrete ad deterministic industrial process environment, the corresponding protocol dissectors are required to represent the process traffic as alphabet-encoded string and collect the transition intervals. The transition profile and interval profile modeling are unaffected and can be successfully extracted. As for the GNN
architectures for process behaviour analysis, the size of the industrial network could impact the computational performance.

**Outlook.** The Suffix Tree algorithm can be substituted with better memory-efficient Suffix Array to extract the *transition profile*. The GNN architectures that are capable of learning from the *dynamic graphs* or *spatial–temporal graph* such as Spatio-Temporal Graph Convolutional Networks (STGCN) [Yu17], Temporal Graph Network [Ros20] can be employed for Graph-based process data analysis and anomaly detection in industrial production.
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<td>AC</td>
<td>Access Control</td>
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<td>APT</td>
<td>Advanced Persistent Threats</td>
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<td>AR</td>
<td>Application Relationship</td>
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<td>ARP</td>
<td>Address Resolution Protocol</td>
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<td>Federal Office for Information Security</td>
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<td>CAN</td>
<td>Controller Area Network</td>
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<td>Data Confidentiality</td>
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<td>Deep Graph Library</td>
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<td>DNA</td>
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<td>Discrete-Time Markov Chain</td>
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