# AI-driven Predictive Manufacturing for Genvia

*Infonum Project*


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# Contents


**1 Introduction** **3**

1.1 Context . . . 3

1.2 Introduction to Genvia: Our Esteemed Client . . . 3

1.3 Hydrogen Fuel layer Operation and Production . . . 4

1.4 Project goals . . . 5

1.4.1 Traceability: Streamlining Manufacturing Operations . . . 5

1.4.2 Durability: Machine Learning for Predictive Maintenance . . . 6

1.5 Project Data Playground . . . 6

1.5.1 Traceability Segment . . . 6

1.5.2 Durability Segment . . . 6

**2 Project Organisation and Task distribution** **7**

**3 State of the art** **8**

3.1 Traceability . . . 8

3.2 Durability . . . 9

**4 Key Analysis and Justifications of Technical Choices** **9**

4.1 Traceability . . . 9

4.2 Durability . . . 10

4.2.1 Signals pre-processing . . . 10

4.2.2 Prediction Model Construction . . . 11

**5 Implementation details** **13**

5.1 Traceability . . . 13

5.1.1 Automation of Manufacturing Order Messages Using JSON Templates . . . 13

5.1.2 Linking JSON to Excel Data . . . 13

5.1.3 Streamlining Data Integration with Python Scripts . . . 14

5.1.4 Automated JSON Generation for Substack table . . . 15

5.1.5 Automated JSON Generation for Stack table . . . 16

5.2 Durability . . . 17

5.2.1 Signals Preprocessing . . . 17

5.2.2 Prediction Model Construction . . . 19

**6 Results and analysis** **22**

6.1 Traceability . . . 22

6.2 Durability . . . 22

**7 Conclusion** **23**

7.1 Traceability: Streamlining Manufacturing Operations . . . . . . . . . . . . . . . . . . . . . . 24

7.2 Durability: Predictive Maintenance Through Machine Learning . . . . . . . . . . . . . . . . 24

# 1 Introduction

## 1.1 Context

The need to address climate change is increasingly urgent, as demonstrated by recent data. According to the graph below [1], the Earth's average surface temperature in 2023 was the highest on record since record-keeping began in 1880.Overall, in 2023, Earth was approximately 1.36 degrees Celsius warmer than the pre-industrial average of the late 19th century (1850-1900). Additionally, the ten most recent years have been recorded as the warmest.

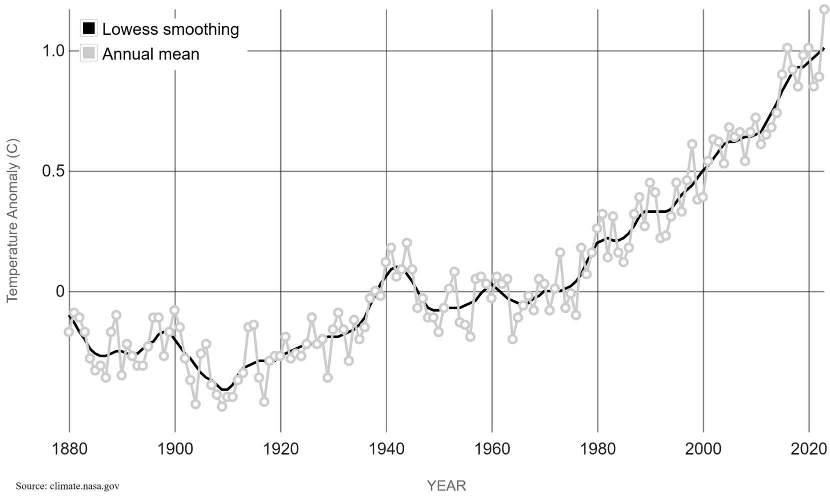



Figure 1: Global land-ocean temperature index

Given this unprecedented climate change, the transition to clean energy sources is imperative. Clean hydrogen, in particular, emerges as a transformative solution for decarbonisation, offering zero-emission energy across various industries and sectors. Its versatility makes it applicable to transportation, industry, and power generation, significantly reducing reliance on fossil fuels and mitigating greenhouse gas emissions.

The importance of clean hydrogen is further emphasized by international collaboration and ongoing research efforts in addressing climate change and advancing sustainable development goals. Clean hydrogen plays a crucial role in shaping a more resilient, equitable, and environmentally conscious global community by fostering innovation and facilitating the adoption of clean energy technologies.

## 1.2 Introduction to Genvia: Our Esteemed Client

Established on March 1st, 2021, Genvia stands as a testament to collaborative innovation, bringing together the expertise of CEA (via its subsidiary CEA Investment), SLB, VINCI Construction, Vicat, and the Occitanie Regional Energy Climate Agency. At its core, Genvia is dedicated to expediting the development and industrial application of CEA's cutting-edge high-temperature reversible solid oxide electrolyzer technology.

This groundbreaking technology is renowned for its exceptional efficiency and profitability in producing decarbonized hydrogen, positioning it as a beacon of promise for a sustainable future. Genvia's vision extends far beyond mere technological advancement; it envisions a landscape where sustainable energy solutions flourish, empowering communities with access to clean hydrogen production, energy storage, and fuel applications.

With key sites at strategic locations across France (Figure 2), the Genvia technology network is accelerating the continuous development of electrolyser solutions at scale that are commercial, cost-effective,

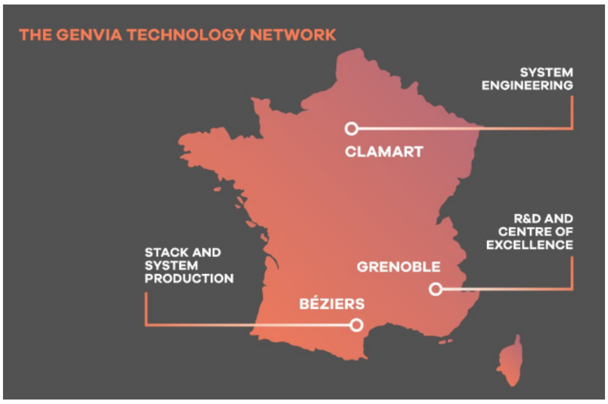



Figure 2: Genvia technology network

reliable and sustainable. By enabling customers to produce hydrogen on site, Genvia solutions also safeguard industry by reducing external dependencies and transportation requirements while protecting local jobs. Our partnership with Genvia transcends the boundaries of our current project. Together, we are poised to achieve remarkable milestones that align with Genvia's overarching objectives. This collaboration underscores the transformative potential when academia and industry join forces, fostering a collective dedication to sustainable innovation and progress.

We extend our heartfelt gratitude to Genvia for entrusting us with this pivotal project, a testament to their commitment to nurturing emerging talent and catalyzing positive change. Together, we embark on a journey towards a future defined by sustainability, innovation, and shared prosperity.

## 1.3 Hydrogen Fuel layer Operation and Production

The first Genvia high-performance electrolyser module is expected to be available for purchase in 2027. In this project we will focus only on the electrolyzers modules, and before diving into the intricacies of our work, we will first introduce briefly the principle of hydrogen electrolyzers.

Hydrogen electrolyzers are devices that use electricity to split water (H2O) into its constituent elements, hydrogen (H2) and oxygen (O2). This process is known as electrolysis and involves passing an electric current through water, causing the water molecules to dissociate into hydrogen and oxygen gas. The principle behind hydrogen electrolyzers lies in the fundamental electrochemical reactions that occur at the electrodes immersed in the water. These electrodes are typically made of conductive materials like platinum, graphite, or other metals that are able to conduct electricity and withstand the harsh conditions of electrolysis.

To facilitate these reactions, an external source of electricity is required. When a voltage is applied across the electrolyzer, it creates an electric field that drives the movement of ions within the water. Positively charged ions (cations) move towards the cathode, while negatively charged ions (anions) move towards the anode. At the electrodes, the ions undergo the respective oxidation and reduction reactions described above. Genvia's hydrogen electrolyzers can work in both Generetor and Motor modes which means that it can either generate Hydrogen from electricity or Generate electricity from Hydrogen.

The Genvia approach allows you to make the greatest use of the heat, chemical and electrical energy present within the electrolysis system. Genvia's *thermally-charged electrolysis* process actively consumes industrial heat so that less additional energy is needed to split the water; reducing the electrical input required to produce each kg of hydrogen. This approach delivers the most energy-efficient electrolysis performance available at scale, with 28% more hydrogen produced for every kWh of electrical energy input.

In terms of production, each module is composed of 75 layers arranged in a stack configuration, or three sub-stacks of twenty-five layers each (Figure 3). Each layer contains an anode, a cathode, and an

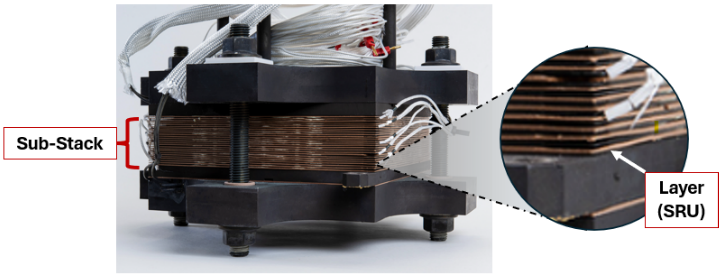



Figure 3: Hydrogen electrolyzer Sub-stack

electrolyte, and these layers are connected electrically in series to increase the overall voltage output of the electrolyzer. Each layer goes through a series of manufacturing steps before the stack assembly step.

Before being put into operation, the assembled electrolyzer undergoes rigorous testing to ensure that it meets performance specifications and safety standards. This may include testing for leaks, electrical continuity, gas purity, and overall efficiency. Any defects or issues discovered during testing are addressed before the electrolyzer is commissioned for use.

## 1.4 Project goals

In our final year project, we will work with Genvia to enhance the efficiency of hydrogen electrolyzers on two different aspects:

- Traceability
- Durability

### 1.4.1 Traceability: Streamlining Manufacturing Operations

As explained in the previous section, each part of the stack goes through multiple steps of pre-processing, assembling, and testing. Following each and every one of those details without a proper data structure is a complex task. Our focus on traceability in manufacturing is to automate the generation of Manufacturing Order (MO) messages. These messages include essential details such as item specifications and delivery dates, aiming to enhance operational efficiency and maintain meticulous records of each order's specifications.

In addition to this, our traceability project entails the restructuring of existing data into a knowledge graph architecture. This architecture comprehensively represents each manufactured stack and permits a more efficient way to ingest information into data analysis and data science models. This restructured approach enables a multi-faceted view of the manufacturing process, facilitating insights that were previously unattainable.

The automation process involves meticulous steps such as:

- Data Consolidation & Processing
- Automation of MO Messages

By leveraging this structured approach, we not only streamline the data capture process but also significantly reduce the time spent on manual data entry. This transformation lays the groundwork for advanced data science applications, paving the way for predictive analytics and machine learning algorithms that can drive further innovation and efficiency in our manufacturing operations.

### 1.4.2 Durability: Machine Learning for Predictive Maintenance

Among the risks that can affect the longevity of a hydrogen electrolyzer (when working in electric energy generators mode) is the potential failures. A failure, in our context, refers to a sudden voltage drop in one of the producing layers, this drop does not stop the electricity production entirely but reduces its efficiency. And since the stack's performance is driven by the performance of its least performing layer, the whole stack become inefficient. As for now, Genvia is still lunching thousands hours tests for each production batch representative stack to see if a failure occurs during those tests (where the name durability came from). Recording the output each stack's layer for +3000hrs is very expensive for the company, thus one of our project's goals is to investigate the possibility of predicting failures only from restricted test intervals 500hrs-700hrs and using the measured voltages across each 5 consecutive layers (since it's mechanically difficult to access all the layers voltages).

To comprehensively comprehend and evaluate the behavior of electrolyzer layers, Genvia aims to explore the feasibility of anticipating failures within each layer stack by harnessing statistical machine learning techniques for anomaly detection. This investigation will not only yield a predictive maintenance model but will also contribute to understanding the characteristics of failures and identifying potential root causes. This side of the project will be constituted of 3 main blocks :

- Data Pre-Processing & Analysis
- Model Construction
- Results Validation & Explainability

## 1.5 Project Data Playground

### 1.5.1 Traceability Segment

In the infrastructure of our data-driven traceability process, two pivotal tables within our Excel files lay the foundation: the Substack and the Stack tables. Each serves as a critical data pool, encapsulating the details necessary for a comprehensive understanding of our manufacturing process.

- **The Substack table**[4]: A detailed chronicle of component-specific data, essential for the granular tracking of the product's manufacturing lifecycle.
  - **Traceability**: Captures work orders, NCR , part numbers, and revisions.
  - **Operational Details**: Logs the initials of the operators, the specific equipment used, and the commencement dates for assembly.
  - **Testing and Quality Assurance**: Details testing parameters like fuel and air pressures at multiple checkpoints to ensure product integrity.
- **The Stack table**[5]: This table complements the Substack table by documenting the assembly and validation stages of the full stack components in the manufacturing process.
  - **Assembly Traceability**: Includes work orders (OF STACK), NCR, part numbers, and revision details to ensure each stack is traceable back to its origins.
  - **Operational Details**: Records the initiation of the assembly process, the operators involved, and the specific testing stations used .
  - **Quality Control Metrics**: Details the measurements of seal integrity and pressure differentials during static and dynamic testing phases, crucial for validating the stack's quality.
  - **Comprehensive Final Checks**: Captures final assembly details such as planeity checks and post-testing measurements, solidifying the stack's readiness for deployment.

### 1.5.2 Durability Segment

In addition to their innovative and green products, Genvia had also a futuristic vision that values the data driven approaches and machine learning potential by incorporating data collection methods in each and every step of the manufacturing and functioning processes.

| SUIVI SOUS-STACK 25-200 200cm² GTRA-0010-02 | | |
|---|---|---|
| OF SUB-STACK | NCR | Part Number |
| MO-GVFR-000002521 | NCR0001251/1277 | |
| MO-GVFR-000002522 | NCR0001315 | |
| MO-GVFR-0000GEX39 | | |
| MO-GVFR-000002627 | NCR0001316 | S-025-200-04 |

Figure 4: Segment of the Sub Stack table

| SUIVI STACK 3*25-200 200cm² V1.2 GTRA-0010-02 | | |
|---|---|---|
| OF STACK | NCR | Intiales |
| MO-GVFR-000002081 BIS | NCR0001079 | AD/YD |
| MO-GVFR-000002081 | NCR0001079 | |
| MO-GVFR-000002171 | NCR0001114 | LP |
| MO-GVFR-000002244 OLD | NCR0001207 | GL/AD |
| MO-GVFR-000002244 OLD 2 | NCR0001207 | GL/AD |
| MO-GVFR-000002244 OLD 3 | NCR0001207 | LP |
| MO-GVFR-000002244 OLD 4 | NCR0001207 | DS |

Figure 5: Segment of the Stack table

- On the manufacturing level, Genvia gathered all the information about each part of the electrolyzers stacks in a primitive format, that will be later the ground of our first automation tests.
- On the electrolyzers durability level, Genvia set the laboratory conditions to record and collect the output voltage data from multiple stacks. For each stack we have the time series of voltage for the 75 layer. We dispose of two datasets, Brhystol's CEA dataset that contains labeled data (where the failure is captured in the recordings) recorded for a total of 3000hrs with the failure at the end of this duration. In Brhystol dataset, the failure occured in the layer $N°2$ at $t \approx 2800hrs$. On the othe hand, Grenoble Genvia's dataset contains unlabeled signals with 800hrs duration, where we can test our approaches and try to predict already the layers with high failure probability.

**Remark**: The numerical values in this report are hidden for confidentiality reasons.

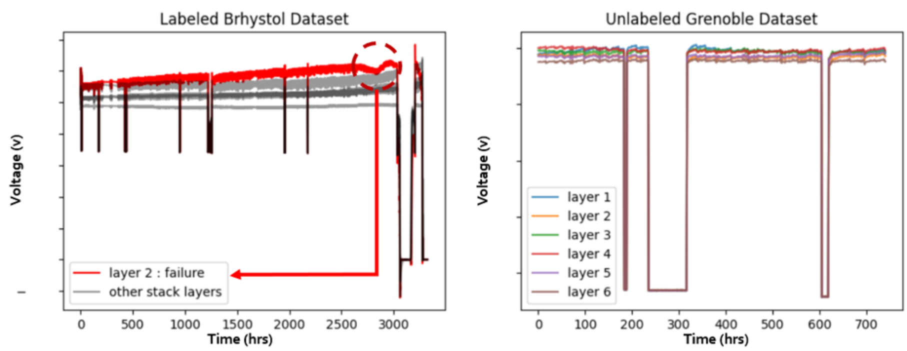



Figure 6: Example signals from both datasets

## 2 Project Organisation and Task distribution

The organization of our project has been meticulously structured to foster clear communication, continuous progress, and collaborative decision-making. Central to this structure are our weekly meetings with Alessia, which serve not only as checkpoints to track our project's advancement but also as vital forums for deliberation on significant decisions. These sessions are crucial, providing an opportunity for every team member to contribute their insights, challenge ideas constructively, and ensure we're moving in the right direction with well-founded reasoning.

Adopting a methodical approach to our workflow, we operate in three-week iterations. At the culmination of each cycle, we engage in an extensive review session with all the members of the team. This is not merely a routine progress check; it's a deep dive into what we've achieved, meticulously analyzing the results of our efforts. These iteration conclusions are characterized by their collaborative nature, welcoming diverse expertise and promoting open-ended inquiries. This approach allows us not just to celebrate our successes but to critically evaluate our strategies, refining our methods and learning from the outcomes to enhance the subsequent phases of our project. Through this organized and reflective process, we ensure continuous improvement and alignment towards our collective goals.

For the task distribution and collaboration within the Durability Traceability project, our approach was highly collaborative and aimed to leverage the strengths and expertise of each team member effectively. Here's a breakdown in bullet points, highlighting the division of labor and the collaborative dynamics between us.

- **Oumaima Chater's Focus on Traceability:**
  - Led the development and implementation of traceability mechanisms.
  - Ensured the project's traceability components met the required standards and objectives.
- **Salahidine Lemaachi's Concentration on Durability:**
  - Spearheaded efforts to analyze and integrate durability features into the project.
  - Worked on developing methods to assess and enhance the product's longevity.

Despite a clear division of tasks, we both remained deeply engaged across all aspects of the project, ensuring a robust exchange of ideas and support that fostered a dynamic and inclusive work environment. This concerted effort allowed for the full spectrum of individual expertise to be harnessed, significantly benefiting the project beyond the confines of designated roles.

The project's workflow was designed to encourage the cross-pollination of ideas, facilitating an environment ripe for continuous improvement and the strategic refinement of our approach. We extended our contributions beyond our primary areas of responsibility, addressing challenges with innovative solutions and efficiency. This collaborative ethos not only introduced a rich diversity of perspectives into the project but also played a fundamental role in solidifying our team cohesion.

# 3 State of the art

## 3.1 Traceability

The concept of traceability in the manufacturing and software development sectors has evolved significantly over recent years. This section synthesizes insights from two pertinent studies to illustrate the current state of the art in traceability.

The first study [1] emphasizes the critical role of traceability in software project management. The authors underscore that traceability, particularly in complex industrial software systems, is paramount to ensuring the coherence between software artifacts and actual system requirements. The paper details the challenges faced when traceability links are missing or inadequately maintained, leading to lapses in software quality and increased project risks. This study provides valuable lessons by highlighting the necessity of both automated tools and human oversight in maintaining effective traceability systems. The collaborative efforts between industry and academia, showcased in the study, are exemplary in overcoming these challenges and demonstrate how structured traceability can substantially enhance project outcomes.

The second study [2] focuses on the applicability of traceability in manufacturing, particularly emphasizing the use of advanced technologies to track components and processes. The research presents a compelling case for the digitization of traceability systems, advocating for the integration of sophisticated data analytics to not only track products but also to glean insights that could streamline manufacturing processes. The incorporation of digital traceability systems enables real-time monitoring and improved accuracy in data collection, which significantly contributes to the overall efficiency of the production lifecycle.

In light of these studies, our traceability project is at the intersection of these two domains, harnessing the lessons learned from the software sector and applying them to the digitization and automation of manufacturing processes. By implementing a structured JSON-based traceability system that draws on the automation principles outlined in the first study and the digital innovations from the second, our project aims to provide an end-to-end traceability solution that enhances operational efficiency, improves product quality, and lays the groundwork for sophisticated data science applications in manufacturing.

These studies collectively inform the approach of our traceability project, highlighting the importance of meticulous traceability in managing and improving complex systems, whether they be software or manufacturing processes. As we proceed, we are mindful of the challenges and equipped with the insights necessary to navigate them, thus ensuring that our traceability system is robust, reliable, and reflective of the state of the art in the field.

### 3.2 Durability

In the realm of time series forecasting and classification, a myriad of methodologies have evolved over the years, each tailored to address specific challenges inherent in temporal data analysis. Traditional approaches have laid a solid foundation, with techniques like Nearest-neighbor classification with dynamic time warping [5], offering robustness against temporal distortions and variations in data sampling rates .

Kernel methods [6] have also garnered attention for their ability to capture nonlinear relationships within sequential data, providing flexibility in modeling complex temporal patterns. Shapelet-based algorithms [7] have emerged as powerful tools for time series classification, leveraging discriminative subsequences to characterize distinct motifs within time series data, thus facilitating accurate classification across various domains.

Additionally, Tree-based algorithms [8] have proven their efficacy, particularly in ensemble frameworks, by exploiting temporal hierarchies and feature interactions for improved prediction performance. Bag-of-words (dictionary-based) approaches [9], originating from text mining, have found applicability in time series analysis by quantifying temporal patterns into symbolic representations, enabling efficient classification based on similarity metrics.

More recently, the advent of imaging time series and deep learning methodologies has revolutionized temporal data analysis [10], offering unparalleled capabilities in feature extraction, representation learning, and predictive modeling. Deep learning architectures, such as recurrent neural networks (RNNs) and convolutional neural networks (CNNs) [11], have demonstrated exceptional performance in capturing intricate temporal dependencies and exploiting hierarchical structures within time series data, thereby pushing the boundaries of forecasting and classification accuracy to unprecedented levels. These advancements collectively signify a dynamic landscape in time series analysis, where traditional methodologies seamlessly converge with cutting-edge techniques, paving the way for innovative solutions to complex temporal inference tasks.

## 4 Key Analysis and Justifications of Technical Choices

### 4.1 Traceability

In the pursuit of enhancing manufacturing traceability, our project embraced a transformative approach, transitioning from traditional, manual processes towards a fully digitalized traceability system. This journey was marked by the key decisions below, driven by the necessity to manage an ever-growing volume of data effectively and to lay a foundation for advanced data analysis and predictive manufacturing capabilities.

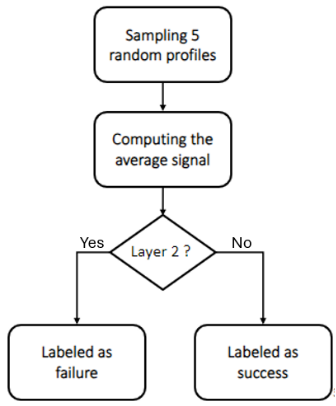
1. **Automation with Python**: Recognizing the limitations inherent in manual and Excel-based data tracking methods, we opted for Python due to its robust libraries and frameworks that facilitate data manipulation and automation. This choice was justified by Python's widespread use in data science and its ability to handle large datasets efficiently, ensuring a seamless transition from data extraction to transformation and JSON creation.

2. **Digitalization Initiative**: Our project's cornerstone was the digitalization of the traceability process, aimed at converting all legacy data into a digital format. This initiative was chosen to overcome the inefficiencies of paper-based traceability and manual Excel entries, ensuring a more streamlined and accurate tracking system that supports real-time data processing and analysis.
3. **Standardization with JSON Templates**: The use of structured JSON templates for Manufacturing Order (MO) messages was a deliberate scientific choice, aimed at standardizing the capture and storage of manufacturing data. This method ensures consistency across manufacturing documentation and simplifies the automation process. The JSON format was chosen for its flexibility, ease of use, and compatibility with web technologies, making it an ideal choice for future integration with other digital platforms and tools.
4. **Foundation for Data Science**: By digitalizing traceability data and adopting a structured approach to data management, our project lays the groundwork for further data science applications within the manufacturing domain. This strategic choice opens up possibilities for advanced analytics, predictive modeling, and machine learning to optimize manufacturing processes and predict potential issues before they arise.

## 4.2 Durability

### 4.2.1 Signals pre-processing

**Mock Profiles Generation:** Because of the technical difficulty that accompanies recording the input voltage of each single layer of the stack in normal circumstances (without laboratory sets & conditions), Genvia's team asked us to rather investigate the possibility of detecting failures from the measured voltage across five consecutive layers which means the averaged signal of 5 layers in the stack. For this reason we chose to start with first step that will mathematically simulate this constraint, this step takes randomly five out of the seventy-five layers, compute their average signal and then label them as failure if one of the five layers is the profile $N°2$ (reponsible for the failure ) and normal otherwise. This way we will also end up with an augmented dataset with more positive and negative instances.




**Signal Cleaning:** As we can observe in figure 6 , the signals, from both datasets, contains some outliers, discontinuities and voltage level differences. For those reasons, we implemented a chain of three cleaning steps, starting with normalization to unify the voltage mean amplitude, filtering to eliminate the outliers and filling to complete the missing parts of the signal where we have no recordings 7. Each step will be detailed in the next section with implementation details.

**Detrending:** Figure 6 shows an obvious difference between the signals evolution between the two datasets, in Brhystol dataset we can see a certain trend or slope, however, in Grenoble dataset, there's nearly no trend and the signals are approximately in the same constant level. This is due to the fact that Genvia also implemented temperature feedback regulation in Grenoble stacks, to stabilize the stack's voltage output. This technique however was not embedded in Brhystol stacks, thus we needed to detrend our training dataset first to be in same conditions as the test one and especially to eliminate the information about failures that may be encoded in the slope evolution (since we do not have access to that info in the test).

**Noise evolution :** Before starting the prediction model implementation, we started with a feature selection analysis that concluded about the importance of the noise feature in our classification task. We analyzed the resulting signals after cleaning and detrending by comparing the distributions of noise levels between the failures and non-failures. The signals were partitioned according to the existing change points that we detected using Binary segmentation technique (BinSeg) [see Figure 8], then the noise levels were computed on each segment separately. As we can see in Figure 8, the two distributions of failure

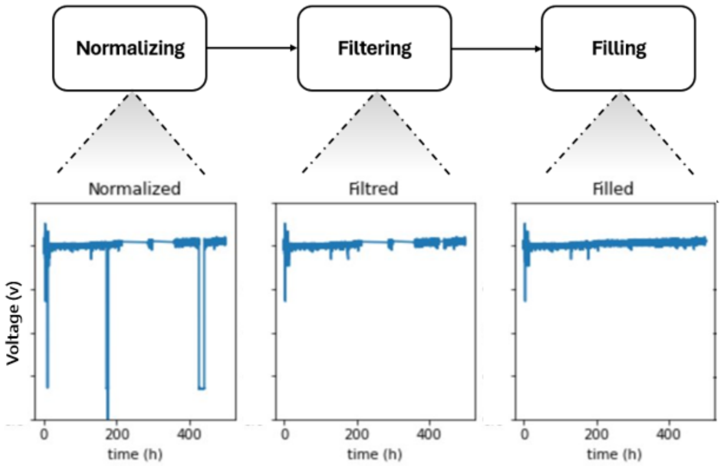



Figure 7: Data cleaning steps

and non failure signals are partially disjoint, which primarily suggests that the noise levels of our signals have significant information to identify failure profiles. Note the overlap region between the distribution of the two classes is very small in this figure because we used the original signals of each layer, however after the averaging operation, the overlap region becomes wider making identifying failures difficult with a simple average noise level classifier.

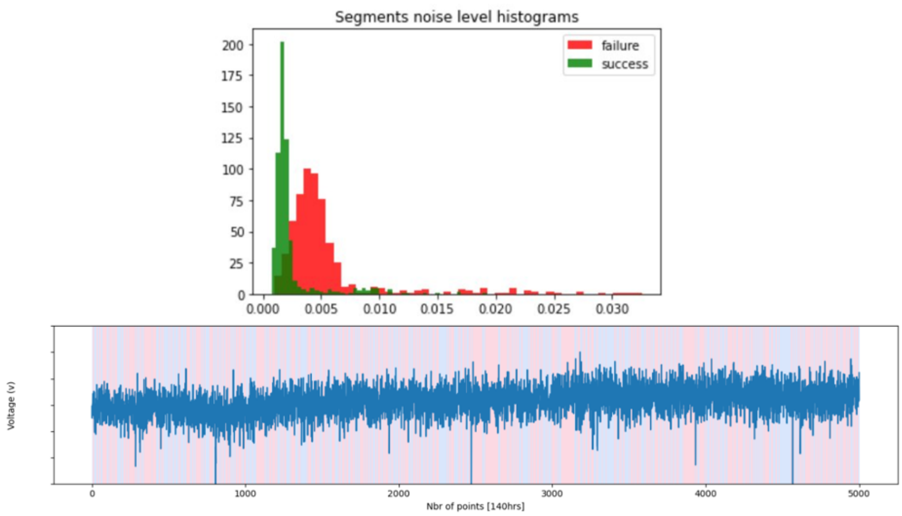



Figure 8: Signals analysis

**Signal to noise evolution:** This analysis motivated us to proceed with a transformation step, that will map each signal its noise level evolution with respect to time and then only consider the resulting signal for the rest of the process (Figure 9). This transformation step will also facilitate analyzing our profile that are very noisy by nature by reducing their dimensionality and inferring clear learnable patterns.

#### 4.2.2 Prediction Model Construction

After completing the pre-processing block, we started our research about efficient anomalies detection models that will fit our problem and requirements.

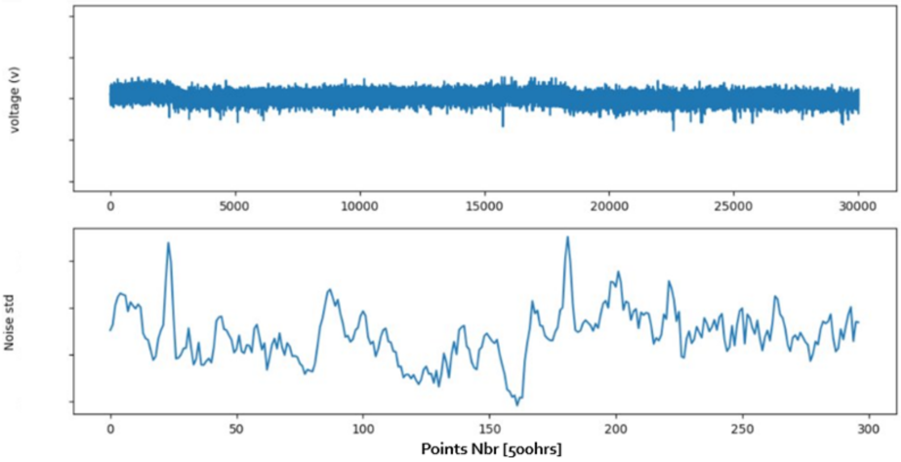



Figure 9: Signal to Noise evolution

- The model should have an unsupervised learning component that help on fitting it on every new stack and take into consideration the possible change of features between different datasets (this change can be caused by the change of tests tools, laboratory conditions and measuring processes).
- The model should enable the possibility of coupling it with a counterfactual explanation module that will helps us understand the characteristics of failure layers, and what could've changed in signal to be labeled otherwise.

In this scope, we were inspired by this work [3] about Counterfactual Explanation for Multivariate Times Series Using a Contrastive Variational Autoencoder. This paper's model had the potential to fulfill all our requirements thanks to the unsupervised nature of contrastive variational autoencoder that enables this model to understand the dynamics of the inputs signals and also the important features responsible for the categories distinction. Moreover, we can conceptualize multiple explainability prototypes on the salient embedding features to obtain the explanation on the reason why an instance was labeled as failure or not. In the context of the paper, the model was used to identify pathological classes using ECG data, and they used simple Multi-Layers Perceptrons for the encoder/decoder and took directly the ECG signals as Inputs/Outputs.

We Tried to implement this method in our project, by training the VAE on our Noise evolution signals for each generated & preprocessed Mock profile , however, the model struggled with generelization when we shift the signals intervals away from the training ones. In addition, the prediction were highly unstable between different executions because our preprocessing contains random components in the filling step, so depending on the inferred random samples that were used, the prediction probability changes with a high standard deviation. For all those reasons we chose to modify the model and choose another input representation of our signals using the following method.

**Imaging times series:**
As we mentioned in the state of the art section time series imaging methods have been increasingly used in time series forecasting and classification context, moreover, it has been proven in many references their efficiency over classical models. The advantage of transforming signal from the temporal-numerical representation to images is having access to the immense potential of convolutional neural networks and other deep learning models. In addition, these transformations offer free features augmentation by representing the signal's patterns and dynamics in 2D images form. In this study, we used three main transformations :

- Gramian Angular Transformation: A Gramian angular field measures temporal correlation by computing the trigonometric sum or difference between all the pairs of angles. When the trigonometric sum is applied, the Gramian angular field is called a Gramian angular summation field, while it is called a Gramian angular difference field when the difference is applied. Let GASF be the matrix of a Gramian angular summation field and then GADF the matrix of a Gramian angular difference field (see example in Figure ). The mathematical details will be explicitly explained in the implementation details section.

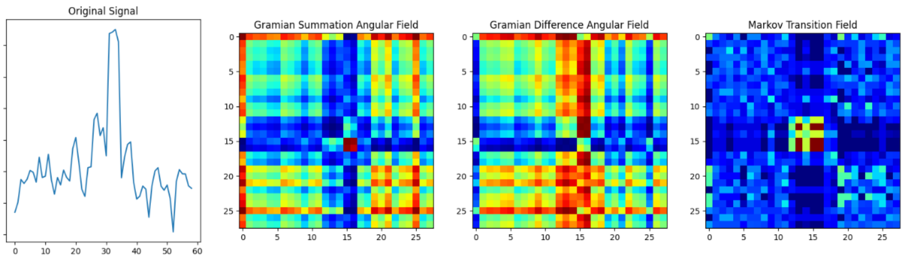



Figure 10: GASF, GADF and MTF imaging examples on one of our signals

- The Markov Transition Field (MTF) transformation converts time series data into image-like representations by symbolizing the data, constructing a transition matrix based on sequential transitions between symbols, normalizing the matrix, and reshaping it into an image format. MTF captures temporal dynamics, reduces dimensionality, offers interpretability, and is flexible for various types of time series data. Like the Gramian Angular Field Transformation (GAF), MTF enables the application of image processing techniques and machine learning models for analysis, making it valuable for tasks such as anomaly detection, classification, and forecasting.

Each one of those imaging transformations will add complementary information about the signal to better describe it.

**Modified Variational Auto-Encoder:**
The modification of data input structure induced naturally a change in the VAE's architecture. To adapt to this change we used Convolutional Neural Network for the encoder block. However, for the decoder, instead of reconstructing the same input images, we reconstruct the corresponding time series signal that was used to create those images. This choice was made to keep the advantage of counterfactual explanation that can be deduced from the decoder part of the VAE (explanations directly on the original signal are naturally interpretable compared to explanations on 2D images). This will also create a type of pretext task to pre-train the VAE model on understanding the nature of our data images and reconstruct the original signals. In the next sections we will explain in details the training strategy of our model as well as the obtained performance results.

# 5 Implementation details

## 5.1 Traceability

### 5.1.1 Automation of Manufacturing Order Messages Using JSON Templates

To simplify the creation of Manufacturing Order (MO) messages, we use a specific JSON template [1] from the 'gv.mfg.mdl' library, a tool created by Genvia's industrial/digital team. This template provides a comprehensive framework for organizing essential data attributes required for MO messages. It guarantees consistency across our manufacturing documentation and significantly automates the documentation process. The template is designed to capture a range of information, from order details such as IDs and product descriptions to a traceability chain that includes every component, serial number, and manufacturing step. This integration highlights our dedication to achieving precision, consistency, and efficiency in documenting manufacturing operations.

### 5.1.2 Linking JSON to Excel Data

This enables smooth translation of data from Excel to JSON. This section ensures that there is a direct correspondence [see table 1 below] between the attributes of the JSON template and the specific

```
{
  "header": {
    "messageID": null,
    "messageType": "Response",
    "reason": "End",
    "messageSchemaVersion": "1.0.8",
    "messageSchema": "OperationMessage",
    "parentOrderID": null,
    "orderType": "ManufacturingOrder",
    "operation": {
      "operationID": "OP00000183",
      "operationNumber": "",
      "operationDescription": "",
      "operationType": "",
      "operationDuration": null,
      "operationDurationType": null
    },
    "manufacturingOrderID": "MO-GVFR-000000082"
  },...
}
```

Listing 1: a section of the JSON template

information in the Excel columns. The process involves a detailed analysis of the JSON templates to accurately source data from the designated Excel columns.

| **JSON's attribute** | **The Excel column** |
|---|---|
| messageID | SUIVI SOUS-STACK 25-200 200c m$^2$ GTRA-0010-02/OF SUB-STACK+"_001" |
| manufacturingOrderID | SUIVI SOUS-STACK 25-200 200cm$^2$ GTRA-0010-02/OF SUB-STACK |
| productID | Traçabilité/Part_Number + "_" + Traçabilité/Revision |
| ... | ... |

Table 1: Example Mapping of JSON Attributes to Excel Columns for the Substack Table

### 5.1.3 Streamlining Data Integration with Python Scripts

Building on the foundation laid by aligning JSON attributes with Excel data columns, we transition to a crucial component of our traceability enhancement efforts: the automation of data integration via Python scripts. This next phase is designed to further streamline the conversion of Excel data into structured JSON formats, ensuring our manufacturing order messages are generated with unparalleled accuracy and efficiency.

- **Data Extraction:** With the mappings established, our scripts proceed to extract the relevant data from designated Excel sheet tabs. This step is foundational, as it converts unstructured or semi-structured Excel data into a format that can be further manipulated programmatically.
- **Data Transformation:** Following extraction, the data undergoes a series of transformation operations. This includes cleansing, formatting, date conversion, string concatenation, and numerical value adjustments. The transformed data aligns with our JSON schema requirements, readying it for the next stage.

- **JSON Creation:** Utilizing the transformed and mapped data, the scripts then populate a JSON template, creating a structured JSON object for each manufacturing order. This object serves as a standardized format for further processing and integration into our systems.

#### 5.1.4 Automated JSON Generation for Substack table

The creation of JSON files for the Substack table is a targeted approach within our broader traceability strategy. This report focuses on certain aspects of traceability that are crucial for tracking the intricate details of our components. The aim is to ensure a focused and detailed analysis within the scope of this report.

**Product traceability:** In the field of product traceability, each sub-stack is identified by its serial number and broken down into its constituent parts, known as layers or SRUs (Serial Replaceable Units). Each layer is essential to the sub-stack's functionality and is meticulously catalogued with its own serial number. This hierarchical approach to traceability allows for tracking of both the final product and its individual components. This is critical because the performance of the substack is determined by its least performant layer.

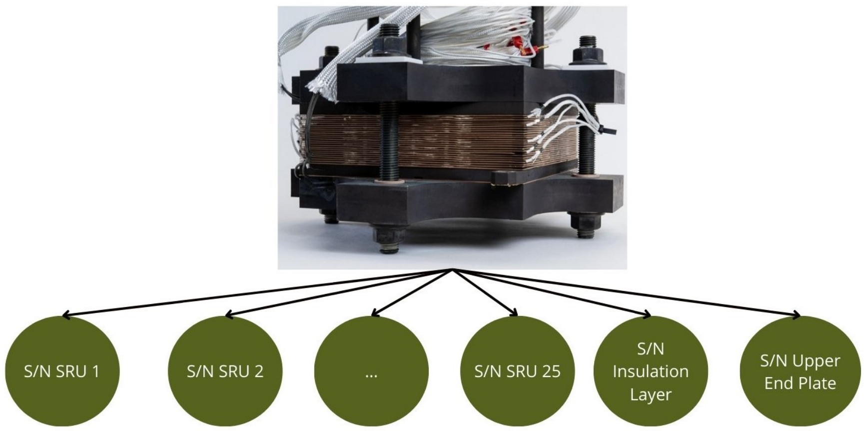



Figure 11: Hierarchy of Sub-Stack IDs

**Process traceability:** When examining the process traceability of the Sub-Stack table, it is important to distinguish between execution and output parameters. Both of these aspects are crucial in providing a complete understanding of our manufacturing process. Execution parameters serve as instructions for our operations, specifying the conditions under which each component is processed. The commands initiate the transformation of raw materials into functional layers of the Sub-Stack. The parameters are identified by the word 'IN' in the column name, as shown below.
In the preliminary stage of data handling, we systematically organize execution parameters by associating them with their specific tests, due to recurring parameters found across various tests. Subsequently, we refine the extraction process by delineating the gas composition and its associated values, directly inferring from the nomenclature used in the column headers. This meticulous approach ensures that each parameter is accurately identified with a descriptive 'parameterID' that encompasses both the test and the gas type, leading to the formation of the final structured dictionaries for 'executionParameters' and 'executionParameterValues'.
After efficiently grouping execution parameters, attention is shifted to output parameters. All column data within each test is encapsulated. This process mirrors the approach with execution parameters. Output parameters are collated under their respective test names to maintain coherence and simplicity in tracking. Following this, data values for each parameter across the spreadsheet's rows are meticulously

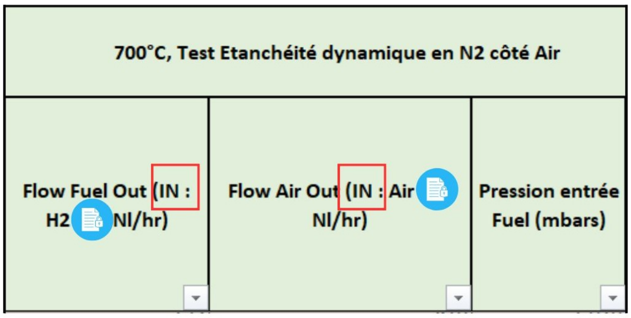



Figure 12: Example of Execution Parameters

```
executionParameters=[
  {
    'parameterID': 'Flow_Fuel_H2_700°C_Test_Etanchéité_dynamique_en_N2_côté_Air',
    'parameterName': 'Flow_Fuel_H2',
    'parameterType': '_Unknown'
  },
  ...
]
executionParameterValues=[
  {
    'parameterID': 'Flow_Fuel_H2_700°C_Test_Etanchéité_dynamique_en_N2_côté_Air',
    'value': '___',
    'valueType': 'String'
  },
  ...
]
```

Listing 2: Example of Execution Parameters and Their Values

extracted. This precise extraction is crucial for creating dictionaries similar to those we created for execution parameters.

These dictionaries are then meticulously crafted to ensure that each entry in 'outputParameters' and 'outputParameterValues' accurately reflects the test results. This preserves the integrity of our traceability data and ensures that every stage of the manufacturing process is recorded and can be reviewed and analysed.

#### 5.1.5 Automated JSON Generation for Stack table

As we expand our traceability strategy, we are focusing on the Stack table. Here, we explore the layers of the Stack, each of which is as important as the previously discussed Substack elements. The approach is identical to the Substack table with a small change in the product traceability section.

**Product traceability:** A comparable method to the Substack table is employed, with the added complexity of requiring comprehensive tracking of each Substack. For every Substack listed within the Stack table, we conduct a cross-reference search in the Substack table. This step is crucial for tracing, and for enriching our dataset with vital supplementary information, such as part numbers and revision histories. It allows us to create a multi-dimensional perspective of each component, ensuring that every aspect of our product is complete, up-to-date, and verifiable. This cross-referencing not only strengthens our traceability framework but also improves the granularity and usefulness of our data for downstream processes, such as quality assurance and lifecycle management.

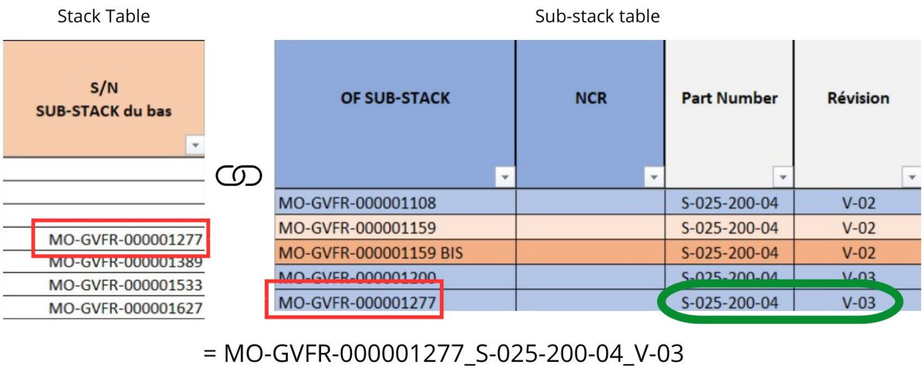



Figure 13: Cross-Referencing Stack and Sub-Stack Tables for Complete Component Details

## 5.2 Durability

### 5.2.1 Signals Preprocessing

**Mock Profiles Generation:** To control the number of negative and positive instances we want to generate, if we want a failure instance, we fix one of the 5 signals to layer $N°2$ signal and randomly select the other four signals, and in case we want a positive instance we randomly select 5 signals (excluding $N°2$). We fixed a number of generated instances to 5000 per stack dataset, devided into 4000 for training and 1000 for testing. The probability to have the same averaged signal repeated is very small and requires a dataset size $s >> 10^8$. In the next paragraphs our dataset will be represented in the following mathematical form:

$$X = (x^0, x^1, ..., x^n)^T$$
$$Y = (y^0, y^1, ..., y^n)^T$$

Where :

- n : the number of generated instances.
- $x^j = (x_0^j, ..., x_p^j)$ : The j-th signal with p data points.
- $y^j \in \{0, 1\}$ : The j-th signal corresponding label (1 if failure and 0 otherwise)

PS : after generation, the signals were chopped to a 500hrs length. However, to increase the robustness of our model and to prevent overfitting, for each signal $x^j$ we sampled 5 shifted signals with the fixed length of 500hrs, the only difference between those signals is the starting instance. We observed that using this temporal shift method instead of a fixed training interval, helped the model to better generalize. So now the total size of our dataset is $s' = 5s = 25000$ instances.

**Signal Cleaning:** After normalization, the signals were filtered using sigma value thresholding by computing the Z score for each signal point $x_i^j$:

$$Z_i^j = \frac{x_i^j - \mu^j}{\sigma^j}$$

Then any points with a Z score $Z_i^j > 1$ was elminated. With $\mu^j$ the mean value of the jth signal and $\sigma^j$ the standard deviation.

Now that our signals are truncated, normalized and filtered we started the missing segments filling. Replacing the missing regions is necessary to the next part of detrending. Under the hypothesis of the noise normality, we chose to compute the normal distribution's mean value and standard deviation in the missing segments surroundings (10hrs recordings), then filling the segment for samples of a normal distribution with similar parameters $(\mu_{new}, \sigma_{new})$ such that:

- $\mu_{new} = \frac{\mu_{before} + \mu_{after}}{2}$
- $\sigma_{new} = \frac{\sigma_{before} + \sigma_{after}}{2}$

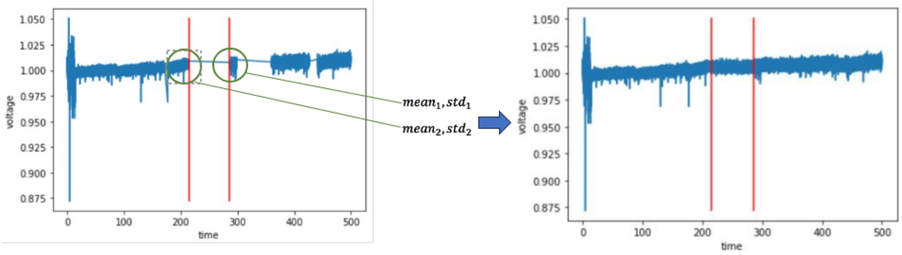



Figure 14: Signal filling technique

**Detrending:** We used linear detrending methods that fits polynomial functions to the signal then substrates the trend from the signal. To choose the polynomial order, we tried orders from 1 to 5 (Figure 15), however since the results of the detrending did not vary remarkably after the first order we chose it as the optimal order.

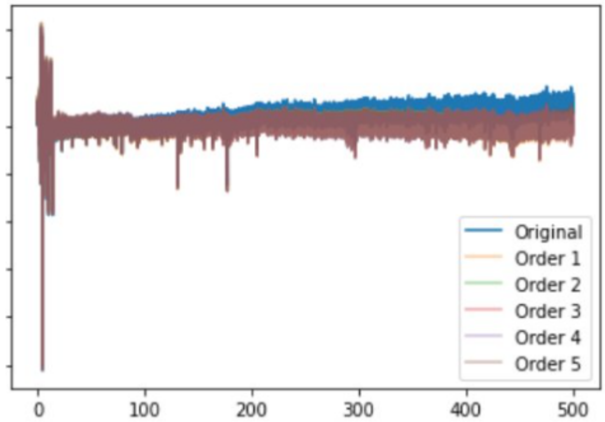



Figure 15: Detrending results for different orders

**Signal to noise evolution:** Using a sliding window, we computed the std on each window using the empirical approximator:

$$\sigma_{win} = \sqrt{\frac{1}{w}\sum^{w}(x_i - \mu)^2}$$

Where w is the size of the window and $\mu$ the mean value of the signal in this window. We can see in Figure 9 that the signal dimension has been reduced, and that's due to the stride parameter we added in the implementation for the window to skip a certain number of points $s < w$ to keep an overlap region between the current and next windows.

**Transformation using Gramian Angular Fields:** To convert the signals into Gramian images, we initiate the process by normalizing the signals to fit within the interval $[-1, 1]$, ensuring their suitability as arguments for the function *arcos*:

$$\forall i \in \{1, \ldots, p\} : \quad \widetilde{x}_i = 2\frac{x_i^j - \min(x^j)}{\max(x^j) - \min(x^j)} - 1$$

The normalized time series $\widetilde{X}$ is then depicted in polar coordinates, where the radius depends on the time points and the angles are determined by the values of the normalized time series:

$$\forall j, \forall i \in \{1, \ldots, p\}: \quad r_i^j = \frac{i}{p} \quad ; \quad \phi_i = \arccos(\widetilde{x}_i)$$

A Gramian angular field gauges temporal correlation by computing the trigonometric sum or difference between all pairs of angles. When the sum is computed, it's termed as a Gramian angular summation field (GASF), and when the difference is computed, it's termed as a Gramian angular difference field (GADF). Let $GASF$ be the matrix of a Gramian angular summation field, and $GADF$ be the matrix of a Gramian angular difference field. The elements of both matrices are calculated using the following equations:

$$\forall j, \forall i, k \in \{1, .., p\} \quad GASF(i, k) = cos(\phi_i + \phi_k)$$

$$\forall j, \forall i, k \in \{1, .., p\} \quad GADF(i, k) = cos(\phi_i - \phi_k)$$

**Transition through Markov Fields:** Initially, a time series $X = (x_1, \ldots, x_n)$ comprising real-valued observations undergoes discretization based on quantile bins. Each $x_i$ is allocated to its respective bin $q_j$ with $j \in \{1, \ldots, Q\}$, where $Q$ denotes the number of quantile bins. Consequently, this process yields a discretized time series with a length of $n$. Considering this discretized time series as observations from a first-order Markov chain enables the computation of the occurrences of consecutive bin pairs. This computation results in a $Q \times Q$ matrix wherein each entry represents the count of transitions from one bin to another.

Subsequently, normalization of this matrix is carried out to convert frequencies into probabilities, generating the Markov transition matrix. The entries of this matrix denote the probabilities of transitioning from $q_j$ to $q_k$ for every bin pair $(q_j, q_k)$.

Let MTF denote a Markov transition field, and $q$ denote the function responsible for mapping real-valued observations of the time series to their corresponding bins. Each entry in the Markov transition field corresponds to an entry in the Markov transition matrix, thus representing a transition probability. $MTF(i, j)$, signifying the Markov transition field entry for the pair $(x_i, x_j)$, represents the probability of transitioning from the bin associated with $x_i$, i.e., $q(x_i)$, to the bin associated with $x_j$, i.e., $q(x_j)$:

$$\forall i, j \in 1, ..., n, \quad MTF(i, j) = P(q(x_j)|q(x_i))$$

### 5.2.2 Prediction Model Construction

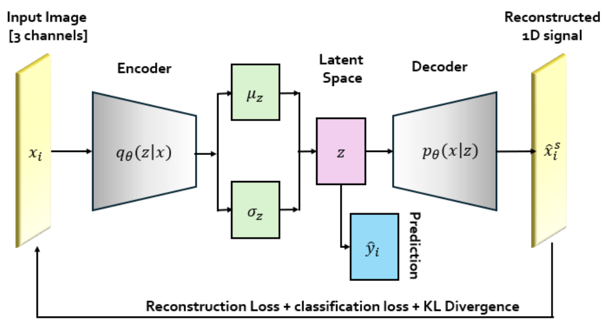



Figure 16: Variational AutoEncoder architecture

VAE are generative models composed of an encoder $q_\phi(Z|X = x)$ which takes the entry x from a high-dimensional space and maps it to a J-dimensional Gaussian with mean vector $\mu(x)$ and diagonal covariance matrix $diag(\sigma^2(x))$, such that :

$$q_\phi(Z|X=x) \sim \mathcal{N}_j(\mu(x), diag(\sigma^2(x)) \qquad [4,5]$$

The decoder $p_\theta(X|Z=z)$ takes a sample z of that distribution as input and generates the associated signal element that was transformed to the input image noted as $\hat{x}_i^s$ . The VAE is trained to optimize the evidence lower bound (ELBO):

$$L_{VAE}(\phi,\theta;x) = E_{Z\sim q_\phi(Z|X=x)}[log(p_\theta(X|Z))] + D_{KL}[q_\phi(Z|X=x)||p(Z)]$$

We have $p_\theta(X|Z)$a Gaussian specified by the decoder, $\mathcal{N}(\mu=\hat{x}^s, \Sigma)$, it is therefore quite natural to write the first term as the MSE between $x$ and $\hat{x}^s$, omitting constants.

The second term in the loss equation is the Kullback-Leibler divergence between $q_\phi(Z|X=x)$ and $p(Z)$. Since the distributions are respectively $\mathcal{N}_j(\mu(x), diag(\sigma^2(x))$ and $\mathcal{N}_j(0, Id_j)$, we can easily compute this term.

On top of the classical VAE losses, we add a cross entropy loss for the classification task that takes the form :

$$L_{classif}(\hat{y};y) = -\frac{1}{N}\sum^{N}(y_j log(\hat{y}_j) + (1-y_j)log(1-\hat{y}_j))$$

**Model Training strategy:**

We observed that when training the VAE model using a direct supervised approach on Brysthol dataset for signals reconstruction and classification, the model fails to generalize on other datasets such as Grenoble unlabelled signals. As you can see in figure 17, the reconstruction errors distribution has shifted from the training and testing one on Brysthol Dataset, and even visually we observed that the signals were not well reconstructed. One advantage our model configuration has is that we can immediately detect such overfitting problems between the different datasets thanks to the reconstruction pretext task. This mismatch problem is often called in the literature as Domain Shift problem. It occurs when the test dataset has some nuisance features that differentiate it with the training dataset.

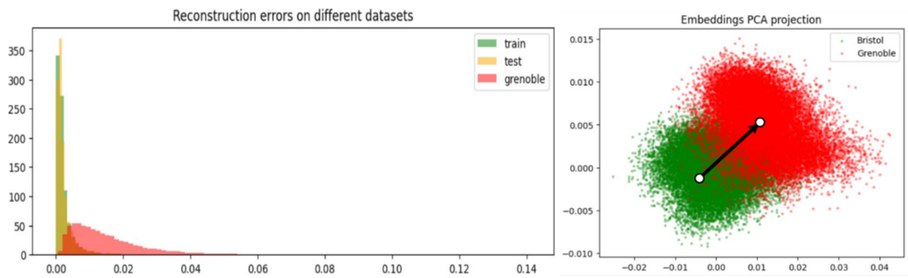



Figure 17: Domain shift problem

In our case, those attributes can be explained by the change of measuring tools, techniques and conditions between different laboratories. We can also visualize it using a Principle Component Analysis on the VAE embeddings, that shows a shift on the general distribution in the latent space.

For those reasons we chose to follow a hybrid strategy between Auto-supervised, Unsupervised and Supervised learning that solve this domain shift problem and adapt to any new stack data (figure 18), inspired from this work [4], where they applied this method to construct a robust speech recognition model that overcomes the nuisance attributes in unlabelled data due to the microphone characteristics change.

First we start by training only the VAE weights (without the classification layers) on reconstructing the signals from both source and target datasets, this will ensure that the model captures the predominant

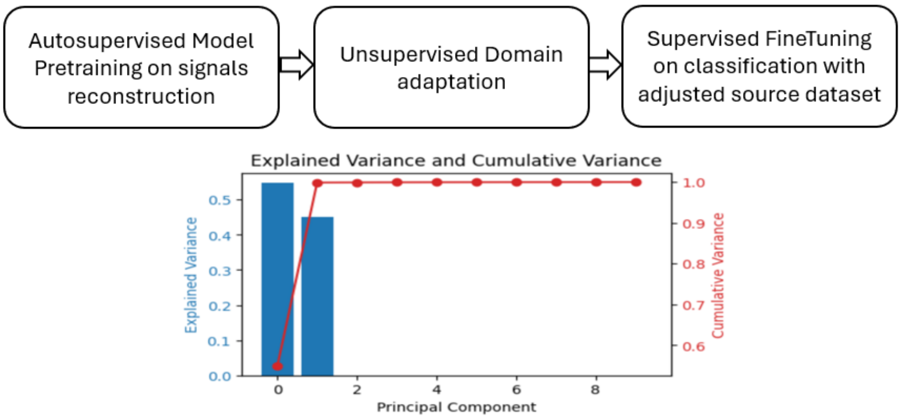



Figure 18: Model training strategy

features in both source and target signals (Brhystol and Grenoble datasets resp). What makes this step possible is the Auto-supervised nature of the pre-training task.

After Pretraining our model, we use PCA on the VAE embeddings for both source and target datasets, to extract the eigen-vectors that explains the variance between the two distributions. Those eigen vectors contain an information about which attributes in the latent space are most correlated with the nuisance attributes that cause the domain shift.

The idea after this extraction is to use it to perturb the source dataset embeddings by augmenting them with similar target attributes, then regenerating those new augmented instances, transforming them into images and using the them as labeled instances for classification fine tuning, this method will ensure that the classification is performed without overfitting on the source dataset nuisance attributes.

An intuitive way to determine and perturb the latent nuisance subspace is to select the first few eigenvectors and only perturb in those directions. They refer to this in the original paper as hard latent nuisance subspace perturbation, since it demands a hard decision on the rank of the subspace. Alternatively, they proposed an approach called soft latent nuisance subspace perturbation, which generates a perturbation vector p as follows:

$$p = \gamma \sum_{d=1}^{D} \phi_d \sigma_d e_d, \quad \phi \sim \mathcal{N}(0,1)$$

where $\phi_d$ is drawn from a normal distribution, $\sigma_d$ and $e_d$ are square root of d-th largest eigenvalue and its associated eigenvector, and $\gamma$ is a hyper-parameter, referred to as the perturbation ratio. It can be observed that the expected scale we perturb along an eigenvector $e_d$ is proportional to the standard deviation of latent nuisance representations along that eigenvector, which is the square root of its eigenvalue $\sigma_d^2$. This approach thus automatically adapts to different distributions of eigenvalues, regardless how many dimensions a VAE learns to use to model the nuisance attributes. In figure 19 we presented a comparative example of the ground truth signal, its reconstruction and its augmented version with the above method.

**Training/Testing datasets details:** For the first pretraining step, we used 20k samples from Brhysthol dataset + 20k sample from Grenoble Dataset. For the classification fine tuning we used Brhystol dataset with 20k augmented samples. The reconstruction was evaluated using 5k sample from Brhysthol + 5k sample from Grenoble. The classification was evaluated using 5k labeled sample from the original Brhystol dataset and 5k labeled sample from the augmented version.

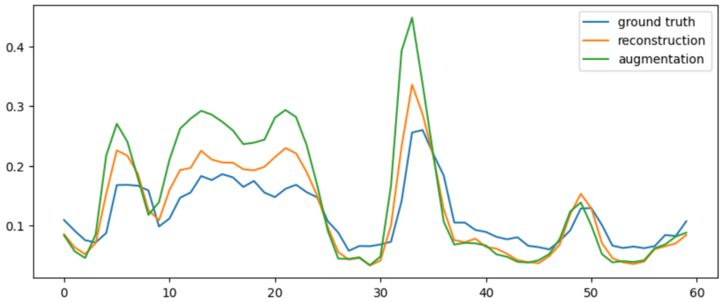



Figure 19: Augmentation example

# 6 Results and analysis

## 6.1 Traceability

This section presents key extracts from the JSON files generated for the Sub-Stack and Stack tables, as depicted in Figure [20]. These snippets demonstrate the successful automation of our traceability data, with each JSON entry providing a detailed account of the manufacturing operations. The creation of these files validates the effectiveness of our digitalization efforts, showing that each manufacturing operation is methodically captured and logged. As shown in the data extracts, we have achieved a high level of precision in documenting the necessary information for thorough traceability and subsequent analysis. This achievement establishes the foundation for advanced data science applications, where well-organized trace data in the form of JSON files enables efficient data processing and analysis.

```
{
  "header": {
    "messageID": null,
    "messageType": "Response",
    "reason": "End",
    "messageSchemaVersion": "1.0.8",
    "messageSchema": "OperationMessage",
    "parentOrderID": null,
    "orderType": "ManufacturingOrder",
    "operation": {
      "operationID": "OP00000183",
      "operationNumber": "",
      "operationDescription": "",
      "operationType": "",
      "operationDuration": null,
      "operationDurationType": null
    },
    "manufacturingOrderID": "MO-GVFR-000000082"
  },
```

SUB-STACK Table

```
{
  "header": {
    "messageID": null,
    "messageType": "Response",
    "reason": "End",
    "messageSchemaVersion": "1.0.8",
    "messageSchema": "OperationMessage",
    "parentOrderID": null,
    "orderType": "ManufacturingOrder",
    "operation": {
      "operationID": "OP00000190",
      "operationNumber": "",
      "operationDescription": "",
      "operationType": "",
      "operationDuration": null,
      "operationDurationType": null
    },
    "manufacturingOrderID": "MO-GVFR-000000303"
  },
```

STACK Table

Figure 20: Partial View: JSON Traceability Segments for Manufacturing Processes

## 6.2 Durability

Our personalized model architecture trained with the hybrid protocol delivered great performance results in terms of signals reconstruction as well as prediction accuracy on test sets :

- Reconstruction MSE: 0.0023
- Classification accuracy (non augmented dataset): 89%
- Classification accuracy (augmented dataset): 91%

After ensuring the good performances of our model, we started testing it on the unlabeled Grenoble signals to infer new failure predictions. We followed the same preprocessing strategy that we used to train and evaluate the model :

Mock profiles generation -> Data cleaning -> Data transformation

In this test we also conserved the composition of each Mock profile, which means the Ids of the 5 layers that were used to construct each profile, this information served us to compute the frequency of each layer (out of 75) in the Mock profiles predicted as failures. We expected the failure layer(s) to be repeatedly used in the failure cluster.

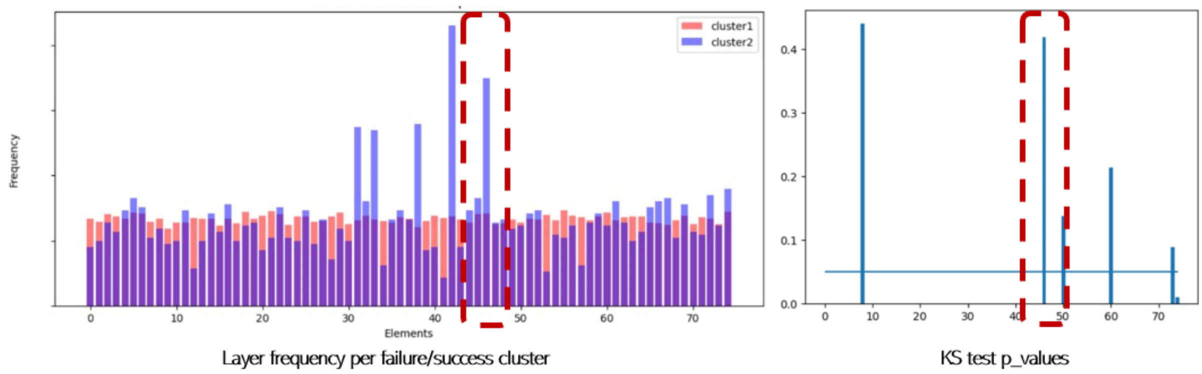



Figure 21: Grenoble test results

As we can see in Figure 21 the cluster 1 corresponds the mock profiles predicted as success, and cluster 2 to the predicted failures. Some layers were more frequent in the layers predicted as failures such as layer 46 and layer 42 with high probabilities (the frequencies can be also interpreted as probabilities if we considered this final prediction as the outcome of many ensemble predictions). To validate those results we performed a statistical KS test that will measure the similarity between each layer in Grenoble Stack and the failure layer in Brhystol dataset in terms of statistical distributions. The right bar plot in Figure 21 confirms the high similarity between the layer 46 with the training failure profile, however the KS test does not detect the similarity between the other layers predicted as failures and our training failure profile, this can be explained by the fact that multiple types of failures can exist and be detected with our model whenever they diverge from the normal behaviour. Nervertheless, more tests should be done to explain the other predictions of our model, this is where the counterfactual explanation module is important because it will enable us to see the motives for each prediction and the responsible parts in the signal to validate all the results.

# 7 Conclusion

This project aimed to enhance the manufacturing operations and predictive maintenance capabilities of hydrogen electrolyzers at Genvia. Through the utilization of state-of-the-art digital and analytical tools, our objective was to optimize production processes and proactively address potential failures. Integration of advanced traceability mechanisms and the application of machine learning for predictive maintenance signify a paradigm shift in the management of hydrogen electrolyzers. This strategic approach is poised to catalyze efficiency, reliability, and sustainability within the hydrogen fuel production domain, marking a significant advancement in the industry landscape.

### 7.1 Traceability: Streamlining Manufacturing Operations

The traceability facet of our project has delivered a substantial upgrade to Genvia's manufacturing operations, focusing on two pivotal areas: digitalization and process optimization.

- **Legacy Data Digitalization:** We've successfully transformed the (sub)stack test records from paper-based archives to a fully digital format. This not only preserves historical data integrity but also enhances accessibility and usability for ongoing and future operations.
- **Traceability Model Enhancement:** Our efforts have refined the existing traceability model, introducing a more dynamic and integrative framework. This revamped model now provides an augmented view of the manufacturing lineage, with granular traceability from the stack level down to individual sub-components.
- **Man-hour Conservation:** The automation of data capture and entry tasks has yielded a significant reduction in manual labor. This streamlining of processes could potentially conserve hundreds of man-hours, redirecting human resources to more critical analytical and decision-making roles.
- **Data Science Foundation:** Perhaps most importantly, our work has prepared the ground for sophisticated data science endeavors. The structured and detailed datasets now available pave the way for advanced analytics, potentially catalyzing innovations in predictive maintenance, operational efficiency, and product development.

In conclusion, our contributions in traceability have not only improved current manufacturing efficiency but also provided a strategic advantage for Genvia.

### 7.2 Durability: Predictive Maintenance Through Machine Learning

In the durability project we succeed to:

- **Prove** the possibility of **failure predictions** only from the noise information of the measured signal across five stack layers.
- **Build** an efficient **model** not only for anomaly prediction but also for **signals understanding** that reconstructs the input profiles with high accuracy.
- Construct a **solid base** for a **counterfactual explanation module** that will help Genvia to understand the nature of mal-functioning problem and why not their probable causes.
- Infer preliminary results for **failure prediction in Grenoble Dataset** that will need to be validated.
- Save enormous **test costs** as well as the **wasted electric energy** for those tests.

Both traceability and durability are crucial to the long-term success and sustainability of Genvia's operations. The traceability segment provides a detailed oversight of the manufacturing process, while the durability segment aims to reduce risks and extend the service life of the electrolyzers. These efforts combine to create a project that not only meets the current needs of the industry but also anticipates future challenges and opportunities.

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