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Time Series Anomaly Detection for CERN Large-Scale Computing Infrastructure

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To my parents and all my educators, teachers and professors that contributed with their passions to the person that I am today.

Abstract

Anomaly Detection in the CERN Data Center is a challenging task due to the large scale of the computing infrastructure and the large volume of data to monitor. At CERN, the current solution to spot anomalous server machines in the computing infrastructure relies on a threshold-based alarming systems carefully set by the system managers on performance time series metrics of each infrastructure component. The goal of this work is to relieve the burden of this complex task and explore fully automated machine learning solutions in the Anomaly Detection field. Moreover, in virtually every real industrial scenario, labeled data to train supervised machine learning methods are unavailable due to their high cost or difficulties in their collection. Therefore our focus is on fully unsupervised Anomaly Detection methods and we explore the current state-of-the-art including both traditional Anomaly Detection ones and also recent successful Deep Anomaly Detection approaches.

In this work we proposed novel formulations of Time Series specific approaches (CNN Forecaster, VAR Forecaster) and adaptations to reuse traditional machine learning methods (LOF, OCSVM, IFOREST, KNN, PCA) and Deep Learning ones (Autoencoder Fully Connected, CNN Autoencoder, LSTM Autoencoder) with time series data. In addition we explore six ensemble strategies to combine the individual algorithm strengths. We then present a comparative study of these 10 individual methods and 6 ensemble strategies on the CERN use case for identifying the best approach for the specific problem's characteristics of the CERN large-scale computing infrastructure. In addition, given the absence of labelled data we put in place an annotation system to make possible to collect two new Anomaly Detection for Time Series datasets representing two different CERN user categories.

The results of this study in terms of ROC-AUC and training time makes a strong point in favour of the traditional methods that for the specific problem at hand work extremely well; on the other hand we also noticed that they tend to be over-performed by deep methods whenever the time

series patterns for normal instances become less trivial. In parallel with the comparative study we also produced an Open Source Proof-of-Concept Anomaly Detection system.

Sommario

Il rilevamento delle anomalie nel Data Center del CERN è un compito impegnativo a causa della vasta scala dell'infrastruttura di elaborazione e del grande volume di dati da monitorare. Al CERN, l'attuale soluzione per individuare macchine server anomale nell'infrastruttura informatica si basa su sistemi di allarme basati su soglie impostati con cura dai gestori di sistema sulle metriche delle serie temporali delle prestazioni di ciascun componente dell'infrastruttura. L'obiettivo di questo lavoro è alleviare il peso di questa complessa attività ed esplorare soluzioni di Machine Learning completamente automatizzate nel campo del rilevamento delle anomalie. Inoltre, praticamente in ogni scenario industriale reale, i dati etichettati per addestrare metodi di apprendimento automatico supervisionati non sono disponibili a causa del loro costo elevato o delle difficoltà nella loro raccolta. Pertanto, il nostro focus è sui metodi di rilevamento delle anomalie completamente non supervisionati ed esploriamo lo stato dell'arte attuale, inclusi quelli tradizionali di rilevamento delle anomalie e anche i recenti approcci di rilevamento delle anomalie basati su Reti Neurali. In questo lavoro abbiamo proposto nuove formulazioni di approcci specifici per serie temporali (CNN Forecaster, VAR Forecaster) e adattamenti per riutilizzare metodi di Machine Learning tradizionali (LOF, OCSVM, IFOREST, KNN, PCA) e Deep Learning (Autoencoder Fully Connected, CNN Autoencoder, LSTM Autoencoder) con dati di serie temporali. Inoltre, esploriamo sei strategie di insieme per combinare i punti di forza dei singoli algoritmi. Presentiamo quindi uno studio comparativo di questi 10 metodi individuali e 6 strategie di insieme sul caso d'uso del CERN per identificare l'approccio migliore per le caratteristiche del problema specifico dell'infrastruttura informatica su larga scala del CERN. Inoltre, data l'assenza di dati etichettati, abbiamo messo in atto un sistema di annotazione per rendere possibile la raccolta di due nuovi set di dati di rilevamento di anomalie per serie temporali che rappresentano due diverse categorie di utenti del CERN. I risultati di questo studio in termini di ROC-AUC e tempo di allenamento costituiscono un punto di forza a favore dei metodi tradizionali che per lo specifico problema in esame funzionano molto bene; d'altra parte abbiamo anche notato che tendono ad essere sorpassati da metodi basati su Reti Neurali ogni volta che i modelli di serie temporali per istanze normali diventano meno banali. Parallelamente allo studio comparativo, abbiamo anche prodotto un sistema Open Source Proof of Concept di rilevamento delle anomalie.

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Contents

Chapter 1

Introduction

Industry devices such as server machines, engines, robots, etc. are the basis of the correct functioning of virtually any complex industrial system (e.g. Data Centre, car production factory, etc.). Also the healthcare sector is increasingly using sensors to monitor the patient's status and robotic environment to improve the good outcome of a surgery operation. The common denominator of all these complex systems is that they rely on the underlying hardware and software to work efficiently and in a safe manner. Unfortunately, the more a system is complex, the more likely it is to present system failures during its lifetime. As a consequence, its failures will inevitably degrade the performance, eventually with a cascade effect on the whole system. Depending on the nature of the system this cascade failure can be translated in a loss of money [1] or a bad outcome for the patient that can also lead to his death in the worst-case scenario [2]. Therefore, in these contexts where we heavily rely on machines, it is crucial to monitor those complex systems and be informed on the status of their components in order to react promptly and avoid bigger losses from late intervention. In fact anomalies in the data contain useful information to reveal concrete hardware or software failures.

1.1 CERN Context

This thesis originates for an internship I conducted at CERN under the supervision of PhD. Domenico Giordano. As part of the *Openstack Cloud team* I had the opportunity to work closely with colleagues responsible for the maintenance (i.e. *operations*) of the Cloud Infrastructure of the CERN Data Centre. Every experiment for High Energy Physics (HEP) at CERN

requires millions, if not billions of CHF of investment [3], therefore every step in the chain that lead to new results for HEP is fundamental. In particular the elaboration and computation of results is crucial and it happens in the Data Centre, which, with a large number of server machines, configures itself as a perfect case of those complex systems just mentioned. Consequently a continuous monitoring of the Data Centre is required to ensure its correct functioning. The primary goal of a monitoring infrastructure is to give a comprehensive and complete view of the system via monitoring dashboards; and this is already in place at CERN with an excellent monitoring infrastructure. A second and even more critical quality of an effective monitoring infrastructure is to promptly inform the user in case of anomalies in the functioning of the complex system at hand. Being able to observe the system in real-time is not sufficient when the number of entities becomes considerably large. In particular we cannot expect to allocate a proportionate number of human resources to manually monitor every entity. For this reason, there is the need for an Anomaly Detection system that can automatically and reliably spot the problems of the system ideally on par or even better than the human expert.
In this direction, the notion of Anomaly is central, and it is often paired with the concept of Outlier. One of the first definition of outlier dates back to 1969: "An outlying observation, or outlier, is one that appears to deviate markedly from other members of the sample in which it occurs" [4]. Back in those days the goal of Outlier Detection was closely linked to the problem of Data Quality, since for a good data mining application the presence of outliers can be often problematic therefore the identification of outlier patterns is functional to their removal from the dataset for a better data mining result. On the other hand, the concept of Anomaly Detection puts more focus on spotting outliers because they represent interesting events that we want to be informed of (e.g. failures). Depending on the meaning behind the outlier in the literature another synonym is Novelty Detection.
In a modern Data Centre structure where the data are in the form of time series the AD task has to consider the discoveries of anomalies across time [5]. Therefore for CERN Data Centre, an outlier intuitively corresponds to an unexpected event, or set of events, that is rare and differs in various ways from the majority of usual events.

1.2 Challenges and Contributions

Given the size of the CERN context with more than $7'000$ physical servers on premise and a monitoring data rate production in the order of terabytes, the CERN Data Centre configures itself as a perfect Big Data scenario. In this context, as part of my thesis and internship, I was responsible for the designing and implementation of a fully-functioning Proof of Concept for an Anomaly Detection system for the CERN Monitoring Infrastructure. To achieve this paramount goal, my thesis work involved two main components as both Data Engineering and Machine Learning Engineering.
In quality of Data Engineer I faced and overcome the following challenges:

1. **Data Preparation**: I prepared and processed the huge volume of data produced by the monitoring infrastructure in a scalable way with Apache Spark.

2. **Infrastructure Design**: I designed, implemented and integrated in the monitoring infrastructure a pipeline to publish the result candidate anomalies in the monitoring platform for visualization, together with a procedure to let the CERN experts label the time series data as anomalous or normal.

3. **Dataset Collection**: I made it possible to collect two new CERN Anomaly Detection Datasets on time series that will possibly be shared with the scientific community allowing scientists to benchmark their methods on the industrially relevant CERN use case.

On the other hand, from the algorithmic perspective the initial lack of labelled dataset for Anomaly Detection at CERN and also the limited human resources available for annotating this complex data excluded the direct application of supervised techniques in a scalable way. Therefore we found natural to investigate fully unsupervised Anomaly Detection methods since the beginning. For the Data Analytics core of the Anomaly Detection System I worked on the following tasks:

1. **Modelling**: I modelled the Anomaly Detection on Time Series problem at CERN and adapted traditional and deep anomaly detection methods that are designed to detect static outliers to work on our time series data (LOF, OCSVM, IFOREST, KNN,PCA, Autoencoder, CNN Autoencoder, LSTM Autoencoder).

2. **Novel usage of Existing Models**: I designed variants of existing models for our specific Anomaly Detection formulation (CNN Forecaster, VAR Forecaster).

3. **Comparative Study**: I compared a pool of selected unsupervised Anomaly Detection methods on the two newly collected CERN dataset on Time Series Anomaly Detection.

The major contributions of this work to the research field include: a comparative study of some of the most used Anomaly Detection methods, both Machine Learning and Deep Learning ones, on the industrially relevant CERN use case, a collection of two new CERN Anomaly Detection for Time Series Datasets and finally an Open Source software implementation of a Proof of Concept for an Anomaly Detection system produced for CERN in the scope of the internship [6].

1.3 Thesis Structure

The thesis is organized as follows:

- In Chapter 2 we give the first details about the CERN cloud computing architecture and them we formally define the problem we address.
- In Chapter 3 we introduce background concepts necessary to understand this research work, then we review literature on traditional and Deep Learning Anomaly Detection methods.
- In Chapter 4 we describe how we use and adapt the CERN infrastructure to annotate and collect the two CERN Anomaly Detection datasets.
- In Chapter 5 we present details about the design of our Anomaly Detection System and how we prepare the data with it.
- In Chapter 6 we focus on the Data Analytics core of the System describing the novel adaptation of previous methods to the time series scenario.
- In Chapter 7 we assess the performance of the evaluated methods, describing the evaluation procedure and commenting on the experimental results.
- In Chapter 8 we summarize the contributions of this work, present our conclusions and suggest possible future research directions.

- In Appendix A we present further details about the collected dataset.
- In Appendix B we collect an extensive version of the evaluation results.
- In Appendix C we present other complementary details about the system in terms of software contribution.

Chapter 2

Problem Formulation

In this Chapter we give the first details about the specific CERN cloud computing architecture and then we formally define the details of the Anomaly Detection problem we address. We conclude with the main assumptions behind the proposed formulation.

2.1 Monitoring Infrastructure at CERN

To accomplish its research goals on High Energy Physics, CERN relies heavily on the computational power of its Data Centre. The computational resources form a Private Cloud and are managed via components of Openstack, the free open standard cloud computing platform. OpenStack provides an Infrastructure-as-a-Service solution integrated with CERN's computing facilities. CERN users can request on-demand virtual machines resources for production, test and development purposes.
At the time of writing, the CERN Data Centre contains 7 487 hypervisors running 45 362 Virtual Machines (VMs) in total.

Virtual Machine: a compute resource that runs in a software environment instead of directly on a physical computer.

Hypervisor: software that creates and runs virtual machines (VMs)" [7]. It is sometimes also called virtual machine monitor (VMM). In this work we also equally refer to an hypervisor with the terms: *server*, *host*, *machine*.

Those machines run either computations for the various physics experiments or applications and services developed by CERN users to maintain CERN internal IT services. In both cases a malfunctioning of those servers can degrade the quality of service for its users. As a consequence CERN invested considerable amount of resources in making sure that its Data Centre can run as smoothly as possible. The main Business Unit created for this specific task in 2016 is the Monitoring Team from the IT Department whose mission is to "collect, transport, store and process metrics and logs for applications and infrastructure" [8]. To provide an effective Monitoring Infrastructure, the Monitoring Team installed a system statistics collection daemon named Collectd on every single hypervisor.

Collectd: system statistics collection daemon that periodically checks some parameters of the hypervisors and store those values in the Monitoring infrastructure acting as a sensor. This daemon is modular thanks to a plugin system that let the system admin decide which parameters to collect in every hypervisor. Some example of plugins are: CPU, Memory and ContextSwitch. Each of this plugins can collect more than one parameters.

Metric: a time series data representing the evolution of a single parameters collected by one Collectd Plugin installed on the hypervisor. In this work we also equally refer to a single metric with the terms: *metric*, *time series*, *plugin*.

Definition 2.1.1. Time Series: is an ordered sequence of numerical data points $\vec{a} = \{a_0, a_1, a_2, a_3, ..., a_t\}$ where the order is determined by the timestamp $\{t_0, t_1, t_2, t_3, ...\}$ in which those data points are observed. It is naturally unbounded and the most recent data point is referred to as a_t.

2.1.1 The Big Picture: Pipeline Architecture

The current configuration of the Monitoring Infrastructure is composed by five consecutive layers or stages, each of them relies on well known open-source technologies:

1. Sources: where the raw data (e.g. metrics, logs, etc) are produced;
2. Transport: that serves as a connector from the heterogeneous data sources to a unified preprocessing engine;

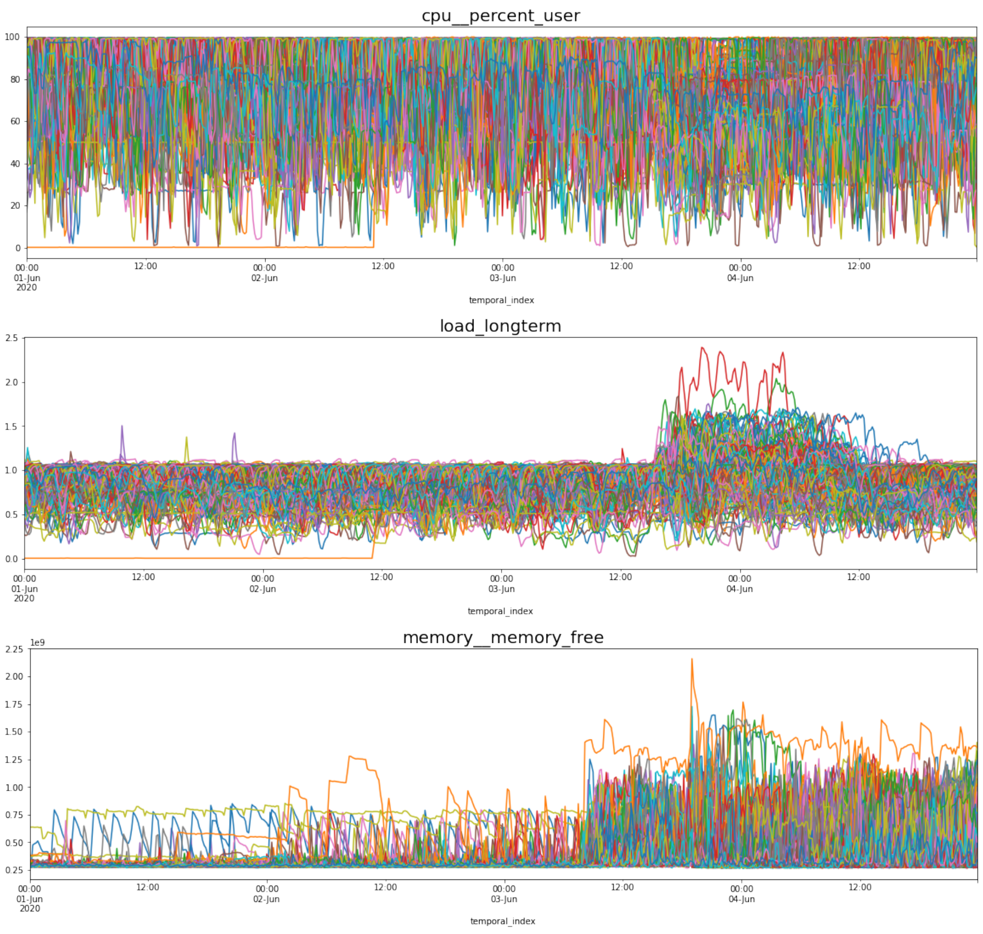

Figure 2.1: Metrics example. Example of three hypervisor's metrics: cpu user percentage, cpu load, memory usage. Data representing the first 4 days of June. Every time series represents a different hypervisor. The hypervisors shown are part of an Openstack Cell devoted to Batch usage (named: Geneva Project 013)

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3. Processing: where data are aggregated and preprocessed thanks to technologies like Spark;
4. Storage: where the processed data are persistently saved for future access;
5. Access: where the data are available to the user for interactive exploration or systematic analysis.

Note that a detailed description the components and technologies I used and how will be given in Section 5.2.

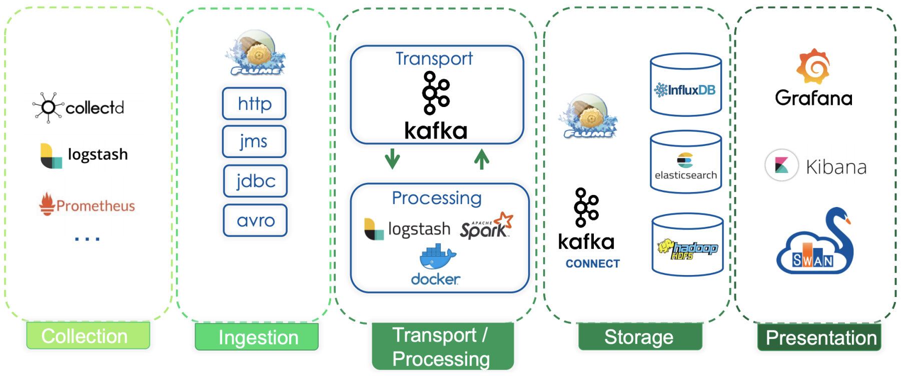


Figure 2.2: Monitoring Infrastructure at CERN. [9]

2.2 Modelling Assumptions

In this section we present the two principal assumptions that let us split the analysis in two main user categories, also called Groups.

2.2.1 Two Main User-Categories: "Batch" and "Shared"

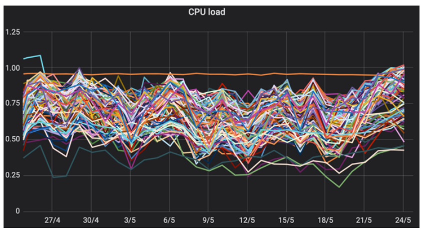
Depending on the computational needs, we have two main user categories. The first one is represented by CERN users or services that are independent from each other and require a relatively low number of hypervisors, whereas the second one consists in physicists that need a large pool of computational resources to elaborate the data from the experiment in a compute intensive way. For the first user category we can assume to have independent and intermittent jobs running on the various hypervisors while in the second case we have jobs that work in a batch and continuous mode showing relatively regular patterns. In Figure **??** we can see the difference between the two categories on the *CPU Load* metric.

Definition 2.2.1. User categories: Every Hypervisor h_i is uniquely assigned only to one target usage:

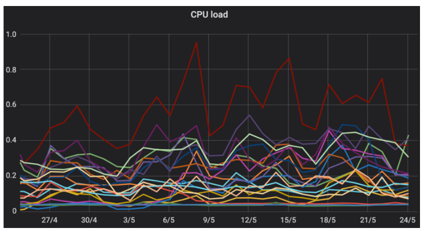
$$\forall h_i \in DC, ((h_i \in S) \vee (h_i \in B)) \wedge (S \cap B = \emptyset)$$

Where DC represent the set of machines in the Data Centre, whereas S represents the set of machines assigned to the "Shared" usage and B to the "Batch" usage.

Set name	**User Category**	**Pattern Usage**	**Objective**
S	Shared by User/Services	Intermittent / Irregular	Maximize the nr of independent jobs satisfied
B	Batch (Physics Experiments)	Regular	Maximize the utilization



(a) *Batch* user category



(b) *Shared* user category

Figure 2.3: Typical CPU load patterns in the two user categories. Every image shows a single group and every line represents the CPU load of a different hypervisors.

2.2.2 Homogeneous Group: same Hardware and Software

To support the various user categories, the compute infrastructure is organized accordingly. The hypervisor dedicated for a common goal are grouped in Openstack Cells.

OpenStack Cell: is a functionality to ease the scaling of an OpenStack cloud in a more distributed way and supports very large deployments. For the scope of this work we will treat it as an aggregate of hypervisors.

More formally we define it as:

Definition 2.2.2. Group (or Openstack Cell):

$$G = \{h_1, ..., h_n\}$$

is a set of n hypervisors with homogeneous Software and Hardware configuration. Moreover they share also the same target usage: batch or shared.

$$(\forall h_i \in G, h_i \in S) \lor (\forall h_i \in G, h_i \in B)$$

2.3 Concept of anomaly

Before diving into the details of our problem formulation, we informally introduce the concept of anomaly. In the spoken language we refer to an anomaly whenever we have something that "is unusual enough to be noticeable or seem strange" (Cambridge Dictionary). We find other more precise description if we refer to the data science literature on the concept of statistical outlier, that is intertwined with the notion of anomaly. According to [10]:

"an outlier is an observation which deviates so much from other observations as to arouse suspicion that it was generated by a different mechanism".

Whereas [11] defines it as:

"an observation [...] which appears to be in- consistent with the remainder of that set of data".

These definitions add two important attributes to our concept of anomaly, respectively the fact that an anomalous observation is normally generated by a different mechanism and that to discover it we always require a peer confrontation with others observations, thus the anomaly is dataset-dependant.

2.3.1 Anomalous Time Series at CERN

In our scenario we are reasoning on time series data, therefore to familiarize with our anomaly detection problem statement we introduce and discuss some typical examples of time series anomaly at CERN.

Figure 2.4 shows some typical anomalous behaviours regarding the metric *CPU LOAD* of the hypervisors in a *Batch* group. The *CPU LOAD* is

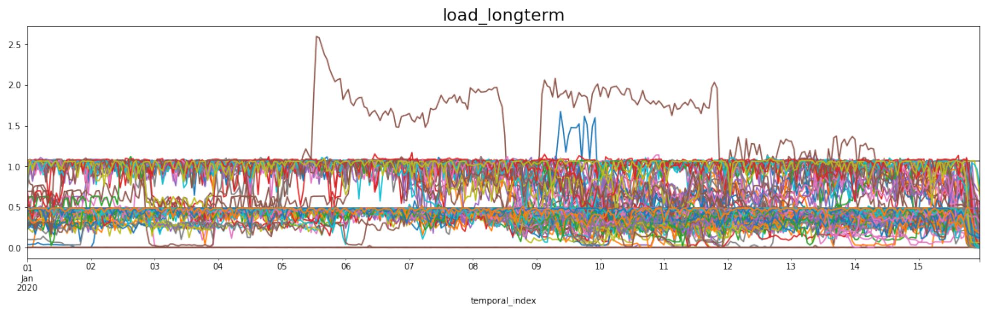


Figure 2.4: Example of anomalies in a Batch group. The brown hypervisor that peaks up to cpu load of 2.5 shows an anomalous behaviour because its load increases above the normal expected behaviour. Other three hypervisors have zero CPU load; that means they are inactive, potentially wasting resource. Ultimately another subset of machines is used only at half of its power with load equals to 0.5.

a measure of the average system utilization during a time period of 5 min, 10 min , 15 min; in this example it is 15 min. *CPU Load* equal to 1.73 means that we have 1.73 runnable processes in the hypervisor, so that on average 0.73 processes had to wait in the queue for a CPU clock (if we assume to be on a single CPU system). The anomalous behaviours can be present with respect to different relative point of reference:

- The past of the same entity. An hypervisor is increasing its activity in a way that never happened in the past. As it can be seen in the Figure 2.4 where some machines go from a CPU load of 1 to 2.
- The behaviour of the other entities. Some hypervisors are having a CPU load of 0.5 and that is strange if compared to the majority of the other machines that instead are fully utilized with load equals to 1, as it is expected in the ideal case for *Batch* group.
- In absolute. An hypervisor with load equals to 0 means an idle resource and therefore a potential waste of resources. In this case it is not necessary to have particular information on the past or the other machines, an idle machine is always bad and we want to identify it.

2.4 Anomaly Detection Problem

Given a Dataset D composed of n samples $D = \{x_1, ..., x_n\}$ where x_i is a multidimensional datapoint $x_i \in R^k$, the goal of Anomaly Detection is to model a binary scoring function $AD(x) : R^k \rightarrow 0, 1$ such that:

$$AD(x) = \begin{cases} 1 & \text{if } x \text{ is anomalous} \\ 0 & \text{if } x \text{ is normal} \end{cases} \tag{2.1}$$

This is virtually every setting achieved with a two step procedure: scoring function followed by the application of a threshold. The scoring function $s(x) : R^k \to R$ assigns to each sample an anomaly score indicating its degree of anomalousness:

$$\forall x_a, x_b \in D, s(x_a) > s(x_b) \text{ if } x_a \text{ is more anomalous than } x_b \tag{2.2}$$

Then we apply a thresholding function $T_c(s(x)) : R \to 0, 1$ to binarize the score, where c is the threshold to discern between normal and anomalous data. The value of the cut-off point c is chosen using a validation dataset so that the false alarms rate stays below a certain desired value.

$$T_c(s(x)) = \begin{cases} 1 & \text{if } s(x) \geq c \quad \text{when } x \text{ is anomalous} \\ 0 & \text{if } s(x) < c \quad \text{when } x \text{ is normal} \end{cases} \tag{2.3}$$

2.5 Time Series Anomaly Detection Problem at CERN

The first step, when working with time series data, is to determine which is the minimal unit of analysis. Since time series data are naturally unbounded streams we adopt the windowing approach and consider for each hypervisor a fixed length window of data.

Definition 2.5.1. Discretized Time Series: given a time series $\vec{a} = \{a_0, a_1, a_2, a_3, ..., a_t\}$, $\vec{d}$ is a derived time series where each data point is a mean summary statistics of the values of $\vec{a}$ in the previous x minutes: $\vec{d} = \{d_0, d_1, d_2, d_3, ..., d_t\}$. Every element d_i summarizes the mean of a disjoint consecutive subset A_i of $\vec{a}$. A_i contains a variable number of elements that were recorded in x consecutive minutes. The start can be fixed arbitrary.

Definition 2.5.2. Univariate Temporal Window: given a discretized time series $\vec{d} = \{d_0, d_1, d_2, d_3, ..., d_t\}$, a Univariate Temporal Window $\vec{w}$ is a vector that represent a subsequence of $\vec{d}$ made of w consecutive data points $\vec{w} = \{d_i, d_{i+1}, ..., d_{i+w-1}\}$, where w is the window length.

We decide to analyse our time series in separate **non-overlapping** temporal windows. Since in our scenario every time series is produced by an hypervisor, we can see the windows as a representation of the health status of that hypervisor. Nonetheless this is only a partial view of our hypervisor because each hypervisor produces m metrics. Therefore we extend our window representation to include also the other time series produced by the same hypervisor.

Definition 2.5.3. Multivariate Temporal Window (or Window): given a hypervisor h and the set D of the m time series metrics it produces $D = \{\vec{d^0}, ..., \vec{d^m}\}$, a Multivariate Temporal Window is a matrix W that has as rows the m Univariate Temporal Windows of h. Note that the univariate windows are *synchronized*, meaning that each column represents the view of the hypervisor h at the same time step for all the m metrics. We refer to it with $W(h)$.

$$W_{m,w}(h) = \begin{pmatrix} d_i^1 & d_{i+1}^1 & \cdots & d_{i+w-1}^1 \\ d_i^2 & d_{i+1}^2 & \cdots & d_{i+w-1}^2 \\ \vdots & \vdots & \ddots & \vdots \\ d_i^m & d_{i+1}^m & \cdots & d_{i+w-1}^m \end{pmatrix} \tag{2.4}$$

Note that: thanks to the discretization procedure it is possible to stack different metrics of the same hyperviosr even if they are produced with different frequencies or in slightly different timesteps, because after discretization each univariate window will have the same length.

If we consider a time window as a sample of our dataset, we go back to the original formulation (Definition 2.1), but instead of representing a generic multidimensional point, our sample represents a Multivariate Temporal Window of a specific hypervisor.

In the next section we translate everything as a problem statement for our CERN specific data centre scenario.

2.5.1 Anomaly Detection in CERN Scenario

Our goal is to detect and identify the windows $W(h)$ of those hypervisors that are showing an anomalous behaviour. We define an instance window $W(h)$ anomalous if it is different enough from the windows observed in the past from that hypervisor and also from hypervisors in the same Openstack Cell. To this purpose we compare various anomaly detection approaches. To reach our goal we are given:

- A Group of n Hypervisors (Definition 2.2.2)

$$G = \{h_1, ..., h_n\}$$

- Training Dataset: sequences of Multivariate Temporal Windows of length w contained in the history of those n Hypervisors with a total length of p discretized time steps.

$$V_{train} = \bigcup_{i \in CW} \bigcup_{h \in G} \{W(h)\}$$

  where CW represents the set indices of all consecutive window segments of length w within p discretized time steps (where $p >> w$).

- Testing Dataset: sequences of non-overlapping Multivariate Temporal Windows of length w referring to those n Hypervisors in a history of f discretized time steps (that come right after the p timesteps used for training). The Multivariate Temporal Windows

$$V_{test} = \bigcup_{i \in NOCW} \bigcup_{h \in G} \{W(h)\}$$

  where $NOCW$ represents the set indices of non overlapping consecutive window segments of length w within f discretized time steps (where $f >> w \wedge f = p$).

We are able now to define our objective:

Goal: *$\forall W \in V_{test}$, assign an anomaly score that is monotonic with the level of anomalousness of that window. The notion of normality and anomalousness are learned from the past history. In addition the score should also let us discern with a simple threshold on it between anomalous and normal windows.*

2.6 Assumptions

The assumption that are behind these problem formulations are:

- hosts in the same OpenStack cells have similar characteristics that can legitimate us to think of them as a "swarm" therefore the deviation from a group behavior could be seen as a good way to spot possible anomalies;

- the discretization procedure of one time series with a mean aggregate every x minutes – where x = **10 minutes** – is discarding high frequency components that are superfluous for the anomaly detection process;

- the selected window length w of analysis – **8 hours** – contains all the meaningful information needed to identify anomalies, or in other words that lower frequencies components not captured by this windows are not relevant;
- the selected history length p – **1 week** – is enough to learn a model of normality.

All the decisions about the length of temporal intervals considered were taken as result of iterative steps of data exploration and domain knowledge coming from CERN monitoring experts. In particular the window length of 8 hours and the granularity of 10 minutes for a single data point, we aimed at filtering out the high frequencies components to reduce the risk of raising false alarms. In addition the number of analysed metrics was fixed at the 11 most used by the domain experts during day to day operations and post-mortem analysis (Table 5.2), exploration on feature selection in such a complex unsupervised setting is left as future work.

Chapter 3

Background

In this chapter we introduce background concepts necessary to understand this research work. After an initial overview of the computing infrastructure scenario, we give review the salient characteristics of both traditional outlier detection methods and Deep Learning approaches, to conclude with an overview of the ensemble techniques available in Anomaly Detection.

3.1 Anomaly Detection for Computing Infrastructures

Nowadays, many applications are deployed on cloud computing platforms such as Amazon Web Services, Google Cloud Platform or Microsoft Azure. In these cases their final users expect a 24/7 availability of the services exposed. However, cloud systems, being specific kind of software systems by themselves, are subject to failures that can result in an anomalous behavior. Beside Cloud platforms and Data Center, every Large-scale and complex online service systems such as global commercial banks [12] and e-commerce such as Ebay [13].

Many of these big players of the industry are investing and researching on methods to cope with anomalies that can arise and undermine their operations. One of the closest use case to the one at CERN is represented by Alibaba [14] that proposed Donut, a Variational Autoencoder approach, but that is focusing only on a single metric and is limited to specific KPI (Key Performance Indicator) metrics. Other examples are represented by Microsoft and Facebook that proposed general methods to work with time series either in the direction of anomaly detection [15] or pure forecasting [16]. Nevertheless they address single time series use case, since it covers a large part of the application, but they overlook the possibility of finding an anomaly in the correlation between multiple timeseries produced by the same entity, what in a Data Centre is represented by an hypervisor monitoring.

3.1.1 Challenges

The Data Center scenario is the perfect representation of a Time Series Anomaly Detection problem. Both Ebay [13] and Microsoft ([15]) identify the following challenges in the area of Time Series Anomaly Detection:

1. **Lack of labels**. Because of the low interpretability of a signal, it is reasonable to believe that it is expensive to find annotators for timeseries if compared to images. Therefore as a consequence, the datasets in the AD for Time Series domain are very much limited to relatively simple benchmark scenarios. Raising the need for the equivalent of the ImageNet dataset for the Time series field [17].

2. **Efficiency and scalability**. Given the size and large-scale of the complex systems under monitoring, it is needed to monitor millions of time series at the same time, therefore the methods used in real industrial application cannot be compute-intensive during the inference step.

3. **Avoid alert spamming**. After all a complex system is monitored and managed by real humans that have limited time to cope with real problem so it is even more crucial to reduce the false positive rate as much as possible and raise the attention only on really crucial matters for the infrastructure.

The first point is the motivator for the effort in putting in place an annotation procedure for anomaly detection, it will be discussed in Chapter 4. Whereas the second point led us focus on relatively simple methods rather that complicated ones, to respect this scalability principle. The last point instead has been reinforced by [15] that envisioned as future work the use of ensemble strategy to provide a more robust anomaly detection service.

Therefore every complex industrial system needs an efficient Anomaly Detection system, as the work of many big player is witnessing. At the same time the alerting has to parsimoniously call for human intervention to avoid spamming and lost of trust in the service itself.

3.2 Algorithms for Anomaly Detection

In this literature review we present some of the main methods in Anomaly Detection including both traditional machine Learning methods and Deep Learning ones; in particular our focus is on fully unsupervised techniques as mentioned in the Introduction. As mentioned in the Problem Formulation (2), virtually any Anomaly Detection algorithm models or learns a scoring function that assign a higher score to abnormal instances and a lower score to normal ones. Therefore in the next part we present every methods together with the way it computes its anomaly score, then the results can be either presented as a rank, starting from the most anomalous sample, or, as mentioned in the problem formulation, we can choose a threshold and highlight only the samples with a score higher than that.

3.3 Traditional Anomaly Detection Methods

We call *traditional* methods those invented before the Deep Learning era: they are generally based on a variety of different key ideas and assumptions. We present the most representative methods used in the literature from that period and also as baselines for current novel methods on Anomaly Detection: K-Nearest Neighbour (KNN) [18], Local Outlier Factor (LOF) [19], Principal Components Analysis (PCA) method [20], Isolation Forest [21], One Class Support Vector Machine (OCSVM) [22].

3.3.1 K-Nearest Neighbour

The K-Nearest Neighbour (KNN) method [18] for Anomaly Detection is based on the following assumption:

Assumption: anomalies are samples that live in regions of the feature space *far* from their closest neighbours.

This is related to the concept of density, therefore samples in areas of low density (absence of close neighbours) are considered anomalies. The closeness of the neighbours is assessed with the euclidean distance $d(\cdot,\cdot)$ in the multidimensional space. The final formula for computing the anomaly score is:

$$s_{KNN}(x) = \frac{\sum_{i=0}^{k} d(x, n_i)}{k} \tag{3.1}$$

where n_i is the i-th closest neighbour of x.

3.3.2 Local Outlier Factor

Local Outlier Factor (LOF) is probably the most known Outlier Detection methods and the first to introduce the locality concept to spot outliers [19]. The main assumption is:

Assumption: anomalies are samples that live in regions of the feature space with low local density (i.e. local with respect to the closest neighbours).

It consists in these main steps:

1. Identify the k-nearest neighbours of every record.
2. compute the k-distance of every record as $k-distance(A)$ coorresponding to the distance of the object A to its k-th nearest neighbor. Usually the Euclidean distance is used.
3. Given the set of neighbours N_k, compute the Local Reachability Density (LRD).
$$LRD_k(x) = \left(\frac{\sum_{neigh \in N_k} dr_k(x, neigh)}{|N_k|}\right)^{-1} \tag{3.2}$$
where $dr_k(\cdot,\cdot)$ is the reachability distance defined as $dr(A,B) = \max(k-distance(B), d(A,B))$ and $d(\cdot,\cdot)$ is usually the Euclidean Distance.
4. Get the LOF anomaly score by comparing the LRD of the current record with those of its nearest neighbours.
$$s_{LOF}(x) = \frac{\sum_{neigh \in N_k} \frac{LRD_k(neigh)}{LRD_k(x)}}{|N_k|} \tag{3.3}$$

3.3.3 Principal Component Analysis for Anomaly Detection

The Principal Component Analysis (PCA) [20] is used to find a linear transformation of your data in such a way that they are projected on directions that maximize the total variance of your data. The procedure to find those direction is equivalent to finding the eigenvalues and eigenvectors of the covariance matrix of your data. The new directions of projection coincide with the eigenvectors just found. Moreover, if we sort the eigenvectors $\vec{v}_1, \vec{v}_2, ..., \vec{v}_p$ in increasing order of related eigenvalues $\lambda_1, \lambda_2, ..., \lambda_p$, we have that the eigenvectors with the highest eigenvalues explain most of the variance, whereas smaller eigenvalues signal direction of low variance in your

data.
In our anomaly detection scenario, it means that if projected the data onto the principal component y_p, we observe high variance of the resulting transformed data, while if we project them onto y_1 they present a small variance, and a continuous behaviour with the eigenvalues in between. The main assumption for using PCA as an anomaly detection technique is:

Assumption: normal data exhibit a small variance if projected to the directions of the eigenvectors related to the smallest eigenvalues, while anomalous data show a high variance on those directions of low variance due to their abnormality.

The intuition is to use this fact, the anomaly score is created by the sum of the deviations of every projected sample with respect to those directions. Following this idea [20] proposes the sum of squares of the standardized principal component scores:

$$s_{PCA}(x) = \sum_{i=0}^{q} \frac{y_i^2}{\lambda_i} \tag{3.4}$$

where $q < p$ aims at selecting only the small eigenvalues and $y_1, y_2, ..., y_p$ represent the projections of record x onto the eigenvectors directions. These projections are also called principal components of the record x.

3.3.4 Isolation Forest

Isolation Forest (IFOR) was presented by [21] and it is among the newest from this pool of traditional algorithms. This method based on random partitions of the feature space with binary split. This binary split is repeated multiple times and it is represented by a binary tree data structure called iTree. The presence of more than one iTree configures IFOR as an ensemble technique. It relies on the main assumption that:

Assumption: anomalies are few and different among themselves and therefore they can be isolated easily even few with random partitions.

During training time we follow the next steps:

1. sub-sample the dataset X with $|X| = n$;

2. construct an iTree by randomly partitioning this sub-sampled dataset X with binary splits. An iTree is build by recursively selecting a random feature of your data and a random value then split the data in two branches. This process stops when either a predefined maximum height of the tree is reached or when the dataset cannot be split further because it contains only one element $|X_l| = 1$ at level l.

Repeat this multiple times and create a predefined number of iTrees, then at test time:

1. Pass each test instance to an iTree and starting from the root of the tree and the attributes of the instance follow the path according to the nodes' splits. Once it reaches a leaf, record the height (called path length);

2. Repeat this for every iTree in the ensemble;

3. Compute the average of the path length for that test instance;

4. Convert this into an Anomaly Score thanks to the following formula:

$$s_{IFOR}(x, n) = 2^{-\frac{E(h(x))}{c(n)}} \tag{3.5}$$

   where:

   - x is the test instance.
   - $E(h(x))$ is the average value of path length in an ensemble of tree.
   - $c(n) = 2 \cdot H(n-1) - \left(\frac{2\cdot(n-1)}{n}\right)$ where n is the number of instances in the dataset X and H is the Harmonic Number approximated via the following equation $H(i) = ln(i) + \gamma$ (Euler's constant = 0.577215).

3.3.5 One-Class Support Vector Machine

As the name suggests, this strategy is a variant of the Support Vector Machine algorithm devised for classification [23, 24]. The One-Class variant [22] aims at estimating the density of the normal data, the basic idea is to find an hyperplane in the feature space that separates the sample normal points from the origin with maximum margin. In this case the origin is taken as representative of the anomalous class. Although this method was initially used in a semi-supervised setting with only normal samples, it can also be used with the soft-margin variation [22] in a complete unsupervised scenario

as we do in our case.
The anomaly score is then computed via the signed distance $sign\_distance(\cdot, \cdot)$ between every point and the hyperplane.

$$s_{OCSVM}(x) = sign\_distance(x, \text{hyperplane}) \tag{3.6}$$

3.4 Deep Anomaly Detection Methods

Given the increasing adoption of Deep Learning in various field, also Anomaly Detection has recently benefited from the application of Neural Networks techniques. A recent study [25] has already confirmed that Deep Learning methods have many potentialities to surpass traditional ones in the such as Network Intrusion Detection field. Further motivations for using Deep Learning techniques are related to two challenges in Anomaly Detection that seem to be solvable only with those methods:

- **need for large-scale anomaly detection**: the increased volume of data requires methods that can process them in a scalable way, regardless of their quantity. Unfortunately many of the traditional methods rely on the computation of distances that in a large dataset becomes computationally demanding.
- **complex data types**: real use cases for Anomaly Detection commonly include the use of image or time series input data. The automatic feature learning capability of Deep Learning techniques becomes extremely useful in these context to avoid the need of developing handcrafted features by domain experts.

3.4.1 AutoEncoder

In terms of techniques used, a recent survey on Deep Learning for Anomaly Detection [26] identifies the AutoEncoder architecture as the main one for this field.

An AutoEncoder consists in a symmetric neural network structure composed by an encoder $e(\cdot) : R^n \rightarrow R^d$ that condenses the input $x \in R^n$ to a lower representation $e(x) \in R^d$ and a decoder $d(\cdot) : R^d \rightarrow R^n$ that is expanding the compressed representation into the output $\hat{x} = d(e(x))$. The objective is then to minimize the reconstruction loss represented by $\sum_{x \in D}(x - \hat{x})^2$, therefore it is trying to learn the identity function. Despite this that trivial objective, a crucial component of its success is the bottleneck in represented by $d << n$ where d is the compressed dimension from which the network has to learn how to reconstruct the input of size n, therefore it has to abstract the salient high level feature of the data in that reduced representation.

The AutoEncoder technique has been used mainly for feature extraction or for removing noise from the input data [27]. In the Anomaly Detection field, their use has been proposed by [28]. The underlying assumption for using this architecture for Anomaly Detection is that an AutoEncoder trained on majority of normal data, will learn how to reconstruct them properly, whereas if we feed it with abnormal data, the reconstruction performance of the network on those inputs will be inferior. The intuition is therefore to use the reconstruction error as a measure for the degree of anomalousness of an input and discriminate between normal data and anomaly.

$$ReconstructionError(x) = \sum_{x \in D} (x - d(e(x)))^2 \tag{3.7}$$

AutoEncoder Variants

Beside the requirements of a general symmetric structure and the bottleneck principle, the rest of the AutoEncoder architecture can be composed in various ways. In fact there exist different variants of AutoEncoder; depending on the main building block we can distinguish the following classes:

- Fully Connected Autoencoder[29]: it consists of a traditional multilayer perceptron architecture with a funnel structure leading to the bottleneck and a symmetric expansion to reconstruct the input.

- CNN Autoencoder [30]: it is based on the fundamental convolution operation that is typically used to work with image data, since its ability of using the information about the neighborhood of pixels. It has recently received lots of attention since its successful application to many high-dimensional and complex pattern recognition problems such as feature extraction [31].

- RNN/LSTM Autoencoder [32]: it is based on a neural network component that can not only take the output of previous neurons in the network as input but it keeps also information in the form of memory from the previous outputs it fired. This is crucial to work with sequence data as in Natural Language Processing or with Time Series inputs. A network including this type of components is called Recurrent Neural Network, and the most recent variant of this unit component are: Long-Short Term Memory (LSTM) [33] and Gate Recurrent Unit (GRU) [34].

3.5 Time Series specific Methods

In the time series literature, our metrics coming form the hypervisors are seen as a stochastic process.

Definition 3.5.1. Stochastic Process: a collection of random variables indexed by some mathematical set. In the time series field this set is typically composed of natural numbers representing subsequent time instants.

The main difference between working with time series data and other kinds of data is that the subsequent time steps in a time series cannot be considered Independent and Identically Distributed random variables (*i.i.d.*). This is the case because previous values usually have some correlation with the future ones. This lack of independence between the variables at different time steps has been modeled and exploited extensively in the literature.

3.5.1 Forecasting Error: Anomaly Detection on Time Series

In the field of Anomaly Detection a way to exploit the time series literature is to create a model that fits the normal data reasonably well, so that at test time if the real new measured data d_t at time t is considerably different from the prediction of our model $\hat{d_t}$, then we flag it as an anomaly. This is also known as *forecasting* or *prediction error* and it is obtained via a distance measure (e.g. euclidean distance) between d_t and $\hat{d_t}$. The assumption behind this kind of models is that a model that fits the majority of normal data will be a good predictor for situation of normality, whereas in abnormal scenarios the real data d_t will be very far from the expectation $\hat{d_t}$ of our model. In the literature we find both traditional and Deep Learning application of this principle [35] [36]; moreover we also mention a previous internal work at CERN is based on it [37].

3.5.2 Traditional Time Series Models

In the traditional time series literature various model families have been proposed to model this dependency between subsequent timesteps:

- Autoregressive - AR(p):

$$d_t = \mu + \sum_{i=1}^{p} \beta_i d_{t-i} + \epsilon_t \tag{3.8}$$

  where p is the order of the model that defines how many past timesteps of the original timeseries we consider for the prediction, μ is a constant representing the mean of the series and ϵ_t is the error represented by white noise.

- Moving Average - MA(q):

$$d_t = \mu + \sum_{i=1}^{q} \theta_i \epsilon_{t-i} + \epsilon_t \tag{3.9}$$

  where ϵ_i are white noise error terms and q is the order of the model that defines how many error terms we consider, μ is a constant representing the mean of the series and ϵ_t is the error represented by white noise.

- Autoregressive-Moving-Average - ARMA (p, q):

$$d_t = \mu + \sum_{i=1}^{p} \beta_i d_{t-i} + \sum_{j=1}^{q} \theta_j \epsilon_{t-j} + \epsilon_t \tag{3.10}$$

  that combines the two models in one, modelling both previous value of the time series and error terms at the same time.

- Autoregressive Integrated Moving Average (ARIMA) where one or more initial differencing steps (”Integrated” part) are used to get a time series that has to certain degree the stationarity property [1]. Then the same formula of ARMA model is applied on the new differenced timeseries.

- Vector Autoregressive - VAR(p): it consists in an Autoregressive generalization designed for multivariate time series.

$$\vec{d_t} = \vec{\mu} + \sum_{i=1}^{p} A_i \vec{d}_{t-i} + \vec{\epsilon_t} \tag{3.11}$$

  where A_i is a m x m matrix with m being the number of metrics and both $\vec{d_i}$, $\vec{\mu}$ and $\vec{\epsilon_t}$ are m x 1 column vectors.

[1]Stationary time series if its properties do not depend on the time at which the series is observed. More precisely, if y_t is a stationary time series, then for all s, the distribution of $(y_t, \ldots, y_{t+s})$ does not depend on t.

3.5.3 Deep Time Series Models

Deep Learning methods in this context make also use of the *forecasting error*. Given a sequence $d_{t-w}, ..., d_{t-1}, d_t$ of the last w timesteps at time t of our time series, we train a Deep model to forecast the timestep d_t given the history $d_{t-w}, ..., d_{t-1}$ as input. The predicted input $\hat{d}_t$ will then be compared with the real available data d_t and the difference between the two is considered as an indication of anomalousness.

We can have two variants:

- CNN forecaster: we have a receptive field sliding on the time series just in the temporal dimension to aggregate information coming from the same time range of different metrics. [35] is representative for the most recent work in that direction, their method consists in a traditional CNN trained on a forecasting objective. Nonetheless it has been trained to detect point anomalies not windows.

- LSTM forecaster: we use the LSTM cell to learn the long term dependencies of a time series to predict the output. A similar work was already done at CERN in this direction by our colleague Ulrich [37]. However, a proper evaluation section on a real dataset with labels was missing.

3.6 Ensemble Methods in Anomaly Detection

Mapping all the methods to a specific problem formulation, therefore making them equivalent in terms of input-output, is beneficial both for evaluating them in a fair way and also for exploring ways of combining them in an ensemble method. In this position paper [38], the authors identified the *diversity* of models as a requirement for the success of an ensemble method.

They reviewed different ways to introduce diversity in the ensemble:

1. Combining the same type of base detector. One technique is feature bagging where each detector uses a different subset of features, an example is [39]. Other alternatives to introduce diversity among detectors consists in using a different subset of the dataset for train or a different parametrization, a prominent example of this type applied to time series outlier detection is represented by [40] that worked with ensemble of RNN Autoencoders. One last way to achieve diversity can be done by introducing a random component during the model learning itself (e.g. isolation forest).

2. Combining different base detector methods and unifying their score as explained in [41].

The intuition behind combining different based detectors is that various modeling strategies capture different characteristics of the data, therefore bringing them together can be useful to mitigate their weaknesses and enhance their strengths, as it has been recently proved by [42] in the context of Explainable AI.

Given the importance of the *diversity* among the single detector used in the ensemble, it is crucial to have a way to assess similarity between those detectors. Unfortunately, as already argued by [43], the AUC-ROC is a metric based on a single final number that does not tell anything about the similarities of different methods. Thus the same authors proposed the Kendall's τ ([44]) correlation coefficient to compare the ordering of rankings.

3.6.1 How to practically combine models in an ensemble

Usually all the AD algorithms returns an Anomaly Score for each sample. This score represents in some way the degree of anomalousness of a certain sample, but unfortunately every algorithm has its own interval and scale of this score, therefore of the first step to merge the prediction of different detectors is to make them comparable. Two natural approaches exist for this purpose:

- **Ranking-based**: for each detector, we order the samples by anomaly score, assign at each sample a position in a ranking system, in which the most anomalous is the 1st and the most normal is the last; then we combine the ranking of the various detectors.

- **Score-based**: for each detector we transform (e.g. translate and scale) the anomaly scores such that the anomaly scores produced by all detectors are in a similar range; then we combine them with an arbitrary aggregation function (e.g. average).

The first approach can borrow techniques from the information retrieval field and some ways to merge the ranking of the various algorithms, but it discard the absolute information on the degree of anomalousness. For example this causes problem when we have only normal data, but according the ranking there will always be a sample that is the most anomalous and if we adopt the approach of flagging as anomaly the first, this might be a false positive by being slightly different from normal data. Another observation in this regard is that if the algorithms is working well, we expect to have a large part of data with similar anomaly scores (i.e. normal data) and few of them with high anomaly score. We would also aim at having the two groups well separated, and we measure this accordance between the order and the ground truth with the ROC AUC.

Combination of ranking

Given the loss of information that we have by converting the score in a ranking, we mention just one of the most intuitive and popular strategy to combine rankings in an ensemble:

- **breadth-first** [39]: it constructs a final ranking merging the single ranking by taking the elements in the 1st position of every method, followed by the 2nd elements of every method, and so on, up to the last elements of the ranking. Given that the methods rank the same elements, we have duplicate copies of the same elements appear multiple times, therefore we drop them by keeping only the first copy of each element.

Although simple, this method has the limitation of being sensible to the order in which we iterate on the various methods; given n AD methods in our ensembles we have $n!$ possible orderings and correspondent final breadth-first results. Due to this characteristic the more the single rankings are different, the more diverse will be the $n!$ final ranking produced by the breadth-first strategy.

Combination of scores

Given the flexibility on aggregating the raw outlier scores, [41] worked in that direction proposing a two steps process to make this scores comparable:

1. **regularization**: to convert the score to a positive number, where close to zero means normal instance while far from it is an anomaly.

2. **normalization**: to scale the scores to a similar interval, so that the algorithms are comparable.

3. **probability conversion (optional)**: to obtain a probability, normalizing in a range [0,1]. This is useful if we want to convert the score in an absolute range that is also more interpretable by the expert. The challenge is that if we train on some data and we set an anomaly score threshold value for which we consider a datapoint d to be an outlier with probability $P(d \text{ is outlier}) = 1$, then it become impossible

to discern between the degree of anomalousness of test-time instances that are above that threshold.

After these steps, we can merge the actual normalized scores form the different methods. We have different strategies:

- **Max**: it take the max score that was assigned to a sample by the various methods; it leads in favour of the most confident method.
- **Min**: intuitively it gives high anomaly scores only if all the methods agree on a high score
- **Average of Maxima**: it divides the methods in groups, takes the max of each groups, and then computes the average among the various groups.
- **Simple average of the scores**: consist in the statistic mean of all the methods. $s_{avg}(x) = \frac{1}{|Methods|} \sum_{i \in Methods} s_i(x)$
- **Cumulative sum**: every sample gets an anomaly score that is the sum of all the anomaly scores assigned to it by the various methods. $s_{cumsum}(x) = \sum_{i \in Methods} s_i(x)$
- **Convex Linear combination**: it consists in a weighted average of the single scores, where the weights are learned by fitting a linear regression using few labelled samples. By ensuring the convex property (i.e. all weights sum up to 1) we enforce the resulting anomaly score to have the same order of magnitude it had before the combination.

The authors [45] reviewed the averaging and maximization combination strategies. From their experimental section they conclude that averaging is a low risk-low reward approach that always reduce the variance. On the other hand, they acknowledged that maximizing can sometimes deteriorate performance but in other case is beneficial to emphasize extra outliers that would have passed unseen with an averaging approach. Nonetheless the scope of their work is limited to ensemble of base detectors of the same species, either LOF or KNN.

Chapter 4

Dataset Acquisition and Annotation

As it is common in industrial settings, companies tend to have an incredibly large data lake but very little of no labeled data. As a matter of fact, this is also the case for CERN, where the time series data are available in large quantities and they are produced at an impressive rate but no one has ever invested time in preparing a curated dataset for the Anomaly Detection task. With these premises, we created an Annotation Pipeline and made it possible to collect an Anomaly Detection benchmark dataset on CERN data with the two following major objectives:

- supporting the evaluation section of this scientific work with experimental results on the actual CERN data;
- giving CERN, as Organization, the possibility to decide to invest in creating new datasets that can enable future work on supervised techniques.

Among the two, the primary aim of this dataset is for benchmarking the Anomaly Detection methods under study in this thesis for the CERN use case; this gives a clearly faster and objective way of judging the anomaly detection system if compared to a qualitative feedback that comes after months of extensive utilization of the system. Nonetheless the second objective is important as well because it makes CERN users think about their monitoring infrastructure as a bi-directional interface that is not only exposing information, but it gives also to the users the ability to input their knowledge in the form of annotations of anomalies, that can function also as a reminder for future colleagues about past problems. We understand that this shift of approach requires time to be fully adopted by CERN users.

4.1 Need for a Dataset: Research Field Perspective

By reviewing a selection of surveys and publication in the field of anomaly detection for time series data [5, 46, 14, 47], we have noticed that every paper validates its new method on its own small restricted dataset. This has been recognized also by the authors of the USR data repository [48] as a crucial lack for the time series/signal processing community. Indeed the scarcity of publicly available datasets is even more evident if compared to other fields like Computer Vision (ImageNet Dataset [17]) and Recommender Systems (The Netflix Prize Challenge [49]) in which the collection of huge and well created datasets gave a clear boost to the respective research communities. In this regard, we firmly believe that the work done for the dataset acquisition during this thesis is the first step to allow the creation of a bigger and more ambitious CERN dataset. Indeed also other world-recognized organization like NASA were able to achieve this in the past [50]. The ambitious aim is to release a dataset that can possibly lead to a less fragmented evaluation section in the various research papers and a more fair comparison among different methods with a hope to advance the research field.

4.2 Extension of Grafana Annotation

Among the technologies present in the Monitoring Infrastructure, Grafana is the platform of reference for the expert to visualize the Time Series data coming form the hypervisors.

"Grafana is a multi-platform open source analytics and interactive visualization web application." Wikipedia

"Grafana allows you to [...] create, explore, and share dashboards with your team and foster a data driven culture." Grafana.com

Since we want to make it possible for the experts to input annotations in an easy and intuitive way, we select the Grafana platform that experts use on daily base for the annotation purpose. As a matter of fact, selecting a familiar tool like Grafana can possibly lead to a faster adoption of annotation practices by the CERN experts.
We can formalize our requirement as:

Requirement: the user should be able to insert "anomalous" and "normal" annotations when looking at the time series of an hypervisor and be able to trace back every annotation to its specific hypervirsor.

4.2.1 "Connecting the dots"

Grafana is organized in dashboards that correspond to web pages where the user can visualise the data in a predefined way. For our particular CERN scenario, a single dashboard collects and visualises multiple time series data belonging to different hypervisors by means of a drop-down menu where the expert can select the hypervisor he wants to inspect. In Grafana, the current value of this drop-down is called Template Variable [1].

Feature 1: With a single dashboard the expert can visualise multiple hypervisors, once at the time, changing the values of the Template Variables.

After careful review of the documentation we found that Grafana provides a native support for point and interval annotation on time series data in the Grafana Annotation functionality [2]. An annotation consists in a start and end time of the interval plus an optional textual description and optional set of keyword that serve as tag for your annotation. Every annotation is dashboard specific and it is saved in the Grafana back-end database. We can therefore query Grafana to have all annotations related to a specific dashboard.

Feature 2: The expert can add interval annotations, that are dashboard specific. Moreover those annotations can be described by tags, and then based on those tags we can then query annotations.

With dashboard specific annotations, if we use the same dashboard to visualise multiple hypervisors, and we put an annotation while inspecting data of one of them, then the same annotation is visible also when inspecting

[1] Grafana Template Variable: `https://grafana.com/docs/grafana/latest/variables/templates-and-variables/`

[2] Grafana Annotation functionality: `https://grafana.com/docs/grafana/latest/dashboards/annotations/`

other hypervisors. In addition, we will not have a way to retrieve all the annotations inserted while the specific hypervisor was visible.

A first possible solution consists in enforcing the user to manually insert tag with the name of the hypervisor it refers to for every annotation, but it is clearly just a first rudimentary solution to the problem, since we have the following drawbacks:

- tedious and time inefficient;
- error prone due to mistyping.

Naive Solution: enforce the expert to add the hypervisor's name to every annotation by hand as tag (tedious and error prone).

Therefore we wanted to fill this gap and find an better solution to ease the work of the expert. Given these premises, we decide to extend the Grafana functionality to automatically append the hypervisor's name as tag with a one-click procedure. We implemented this adding two buttons to the Annotation form (Figure 4.1) in order to automatically flag the annotation with a tag "anomaly" or "normal". In addition the triggered JavaScript code has been extended to append all the template variables of the Grafana dashboard as tags in the Annotation database.

Our solution: it automatically appends info the current value of the template variables of the dashboard (including the hypervisor's name).

Having access to the open-source code of Grafana [3] we could verify that the only needed change was on the client-side JavaScript, leaving the back-end written in GO untouched. The advantage of the developed solution, purely client-side, is to prototype it and enable it as a local override in the user web browser, without having to ask for an entire redeployment of Grafana at CERN. The core code modification is available in Appendix C.1, whereas the complete version is available in our data-analytics repository [4].

Soon we realised that this modification could be of help in all those cases in which we want our annotation to depend not only on the dashboard but

[3]Official Grafana Repo: https://github.com/grafana/grafana

[4]Full code modification available at the following link: `http://go.web.cern.ch/go/Jjb6`

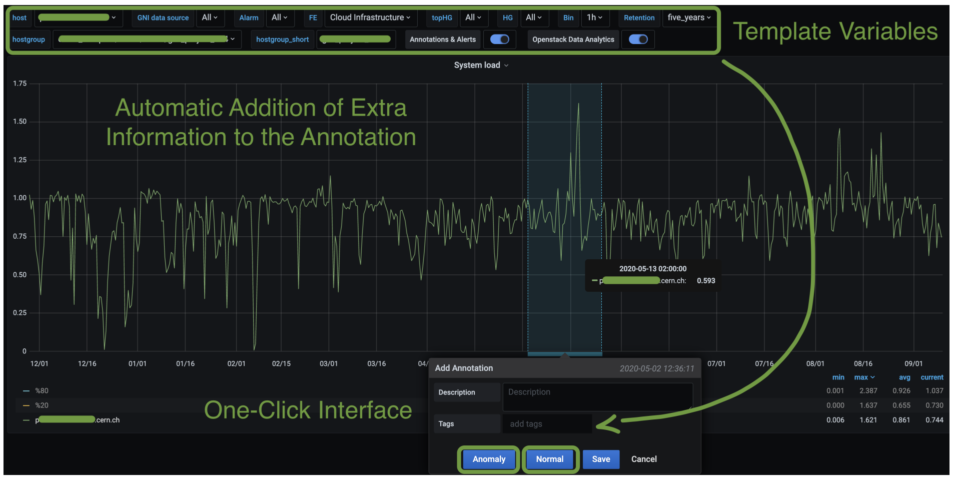


Figure 4.1: Modification introduced in the Grafana Annotation interface. Template Variables are automatically appended as tags.

also on the Template Variables' values that modify the plotted data. Therefore we also started a discussion with the Grafana upstream community for the generalization of our extension for other use cases [5].

4.3 Dataset Creation

Once the annotations are available in Grafana, we can extract them using the Grafana HTTP API [6], to create an offline, standalone labelled dataset. Since we leave to the expert the freedom to decide which interval to annotate without forcing him to annotate always contiguous portions, we had to design how to convert the Grafana annotated intervals in anomaly labels. We evaluated two options:

1. label every data point in the Grafana annotated intervals;
2. divide the Grafana annotated intervals in chunks of of a given time length.

Given our problem formulation, that partitions Time Series in time windows, we decided for the second option. Therefore we converted each Grafana annotation in window annotations of the predefined length of a time window, that generally is 8 hours long, and generates three non-overlapping intervals

[5]Discussion upstream about our Grafana Annotation extension: `https://github.com/grafana/grafana/issues/24674`

[6]Grafana Annotation HTTP API: `https://grafana.com/docs/grafana/latest/http_api/annotations/`

per day: 00:00 - 08:00, 08:00 - 16:00, 16:00 - 00:00. All the possible window annotation configurations and relative annotation resolution strategies are shown in Table 4.1.

Window Annotation Case	**Description**	**Resolution Strategy**
Completely annotated	We have only one type of expert annotation (anomalous or normal) that covers the window entirely.	We label that window as anomalous or normal respectively.
Completely not annotated	The window do not contains any annotated interval by the experts.	We label the window with a special placeholder (e.g. NaN) to represent that we do not have any annotation for it.
Contains only one type of annotation	The window contains one or more annotated intervals of the same type and other portions that are not annotated.	We label that window with the type of annotation(s) present in that window.
Both	The window contains both anomalous and normal annotated intervals.	Regardless of their length, sequence of appearance and overlapping, we label the windows as *mix*

Table 4.1: Declarative description on how we convert the intervals inserted by the expert (with an arbitrary start and end) into window annotations with predefined start, end and length.

4.4 Datasets Description

Given the presence of two clearly distinct user categories we also committed in creating two different benchmark datasets: one for a *Batch* group and one for a *Shared* group. Next we summarize the salient characteristics of the two labelled window Dataset showing the resulting labels distribution given the resolution strategy proposed in Table 4.1. We recall that this datasets are based on the window length of 8 hours and to each window is assigned a label among the following: anomalous, normal, mixed or empty.

4.4.1 Batch Group

For the group of *Batch* hypervisors we annotated 25 of them and the problems exhibited by the machines were related to high or low *CPU load*, *swap* misconfiguration or abnormal memory activity. The interval annotated start from the 13th of February 2020 and end on the 11th August 2020, for a total interval of 180 **days**. In Figure 4.2 we present an overview of the various classes involved, whereas in the Appendix Figure A.1 we present a heatmap giving a visual overview of all the annotations for the *Batch* group scenario.

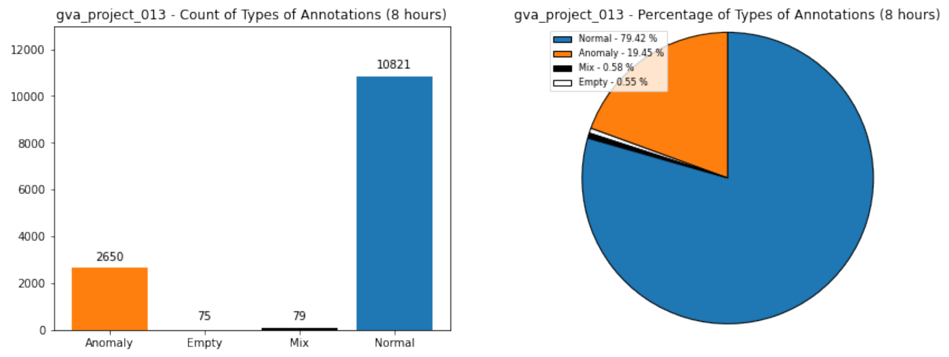


Figure 4.2: Statistics of Annotation Labels for Batch Openstack Cell: blue = normal, orange = anomaly, black = mixed, white = empty interval.

4.4.2 Shared Group

For the Group of *Shared* hypervisors we annotated 73 of them and the problems showed by the machines were related to high or low *CPU load*, abnormal *Context Switch* activity or high *I/O memory* operations. The interval annotated starts from the 1st of January 2020 and ends on the 12th August 2020, for a total interval of 224 **days**. In Figure 4.3 we present an overview of the various classes involved, whereas in the Appendix Figure A.2 we present a heatmap giving a visual overview of all the annotations for the *Shared* group scenario.

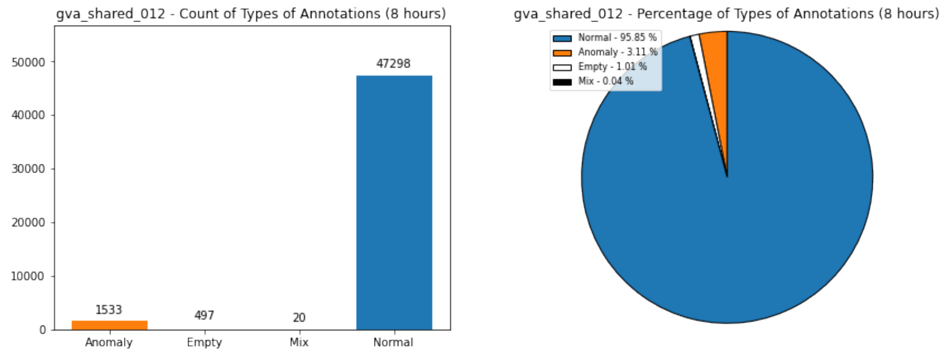


Figure 4.3: Statistics of Annotation Labels for Shared Openstack Cell: blue = normal, orange = anomaly, black = mixed, white = empty interval.

4.5 Artificial Setting Creation

Given the effort required to create the dataset of labeled anomalies, in the first stage we relied on an artificial anomaly setting for the evaluation of the various methods. We exploit the presence of two user categories: *Batch* hypervisors and *Shared* by user/service hypervisors.

The idea is to train the models only on historical data of *Batch* hypervisors and then test them on unseen future windows of data where we inject some hypervisors from the other *Shared* category.

The goal of the algorithm trained only on *Batch* hypervisors is to assign a high anomaly score to the hypervisors coming to the *Shared* category considered another real world generating process, and a low anomaly score to the *Batch* hypervisor sampled form the same generating process.

We took inspiration from the previous work of [51] where they identified few characteristics that a good AD benchmark should have:

1. **Normal data points should be drawn from a real-world generating process.** We achieved this by using real data coming from a different user category.

2. **The anomalous data points should also be from a real-world process that is semantically distinct from the process generating the normal points.** This is guaranteed by the substantial difference in the usage patter of the two categories.

3. **Many benchmark datasets are needed.** This is ensured by the large quantity of data available and the virtually infinite combination of *Batch* and *Shared* data.

4. **Benchmark datasets should be characterized in terms of well defined and meaningful problem dimensions that can be systematically varied.** This can be obtained by varying the metrics as input, that can be up to 170 metrics with 2^{170} possible combinations. For reason of complexity of the problem this option was not pursued, but in alternative we used the similarity between hypervisors of *Batch* and *Shared* cells as an indicator of difficulty.

In practice we also explored one way of controlling the difficulty of the task:

- **Similarity-based injection**. At test time we inject only *Shared* hypervisors that are *similar* to the training data, namely *Batch* hypervisors. This is obtained by means of dot product similarity function between hypervisors' windows. Before computing the similarity we assure that every hypervisor vector is normalized with $norm(\vec{h}) = 1$ where $\vec{h}$ is the vector representing one hypervisor.

- **Standardization of metrics**. In order to make *Batch* and *Shared* more similar and hence increase the difficulty we normalized the input data of both with respect to their own mean and variance so to obtain vectors of metrics with zero mean and variance one. We explored also the option to change only the mean and keep original variance.

Given the availability of real CERN datasets, this artificial setting is used mostly in an exploratory way and the details about the procedure adopted are explained in the Section 7.3.

Chapter 5

Anomaly Detection Solution: System Engineering

Nowadays the main use of the CERN monitoring infrastructure is for (i) real-time inspection of the Data Center status, (ii) threshold-based alarming on the infrastructure components, (iii) and post-mortem analysis of issues after notifications by CERN users. The adopted threshold-based alarm mechanism is in part embedded in Grafana, the CERN monitoring platform, and in part developed in a number of sensors running in each infrastructure entity. In order to increase the level of automation in Anomaly Detection and relieve the system managers from this complex task, a new flexible Anomaly Detection system, based on Machine Learning approaches, is therefore envisaged and prototyped for the CERN Cloud Infrastructure. In this Chapter we explain the main design choices and technologies behind the system, together with a detailed explanation of the data preparation procedure necessary for the Anomaly Detection methods discussed in the next Chapter.

5.1 System Design Challenges

Given the clear necessity of a more Machine Learning aware Anomaly Detection System, the first part of my work at CERN consisted of putting in place a Proof-of-Concept system infrastructure. Indeed no Machine Learning is possible without data, and the challenges at CERN were several including:

- **Big Data processing**: the input data are stored in Hadoop Distributed File System (HDFS) folders and each of them occupy a space in the order of Terabytes (Figure 5.1). Therefore we require a scalable approach to prepare them for our algorithms.

- **Integration with the Monitoring Infrastructure**: the system must be able to communicate with the rest of the infrastructure already in place at CERN, not only in terms of input, but especially in terms of results produced, i.e. candidate anomalies discovered by the algorithms. The system must be able to publish them in the monitoring infrastructure so that the experts can inspect them and can take action.

- **Reproducible analysis**: the entire system must keep track of the operations executed on the ingested data from the start to the end of the pipeline. In this way a candidate anomaly has a clear provenance and the computation that led to it can be reproduced.

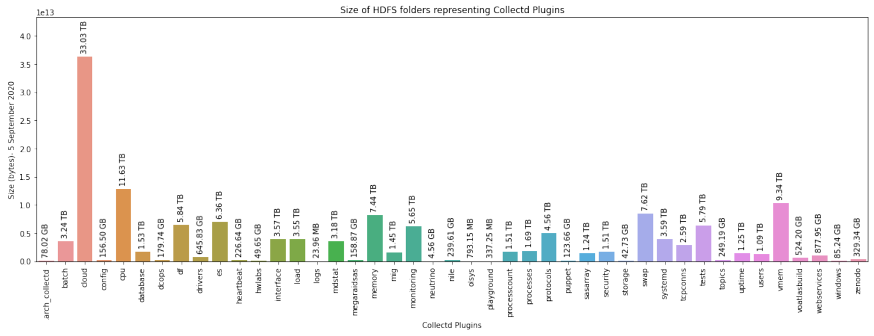


Figure 5.1: Space Occupied by Collectd Plugins. We report the total space occupied by every Collectd Plugins in HDFS. Every plugin is typically containing more than one metrics and for all the hypervisors at CERN since 2018.

5.2 Core Technologies and their Scope

To face these challenges we relied on the following core technologies and solutions:

- **Apache Spark for the Data Preparation**: we employed the CERN Spark cluster to read data from HDFS and pre-process them.

- **ElasticSearch as document storage**: we designed a document format in JSON to store all the information describing a candidate anomalies produced by our system. Details about this format can be found in Appendix C.2.

- **ElasticSearch and Grafana for publishing candidate anomalies**: we designed the above mentioned document format also to be compatible with the visualization platform Grafana, so that the candidate anomalies found by the algorithms are directly visible as annotated intervals in every dashboard that displays the anomalous time series.

- **Grafana Extension for improved interactivity**: we design and implemented an extension to the Grafana platform (Section 4.2) to let CERN colleagues insert their annotations directly on top of the time series they see via the monitoring infrastructure.

- **Apache Airflow to automate the result production**: we use Aiflow to code the tasks performed by the system in a Direct Acyclic Graph (DAG). In this way every step is well documented and it is possible to reproduce the analysis or to automate it by running it periodically on different data as input.

5.3 Anomaly Detection Pipeline

The overall system is represented in Figure 5.2 and it reaches its goals by implementing a process composed of the following steps:

1. Read the data from the Hadoop Distributed File System (HDFS), where the metrics of every hypervisors are safely stored by the monitoring infrastructure (code in Appendix C.3.1);

2. Prepare the data by filtering the group of hypervisors under analysis, aggregating with the mean function in bin of x minutes for creating Discretized Time Series of every metric (Definition 2.5.1) and creating the Multivariate Temporal Window (2.5.3);

3. Analyze the time series window with the Anomaly Detection algorithms;

4. Aggregate the predictions of the single algorithms (optional) thanks to an ensemble layer to increase the confidence on every prediction and reduce false alarms as much as possible;

5. Push the candidate anomalies to ElasticSearch storage and visualise them in Grafana;

At the end of the chain the expert can also annotate normal or anomalous data directly on the Monitoring Dashboard in a faster and easier way thanks to the proposed modification to Grafana (Section 4.2). Moreover, the annotations collected from Grafana can be quickly extracted to create annotated dataset, as those proposed in Section 4.4 by us.

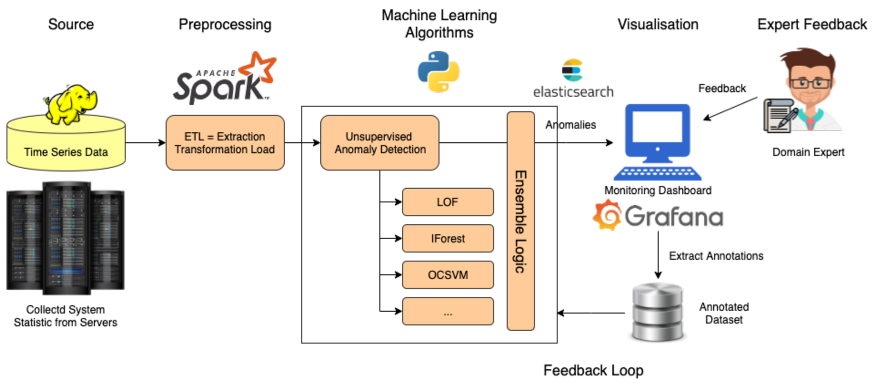


Figure 5.2: Anomaly Detection Pipeline with Expert feedback. Note that the experts can see the result of the algorithms directly in the Monitoring infrastructure via the used dashboard and interact for an easy and fast labelling procedure.

In the context of Figure 5.2 with Feedback loop we refer to the possibility of using the small annotated dataset for other purpose than the mere benchmarking of the algorithms, for example this dataset can be used to develop a supervised ensemble logic layer to combine prediction from multiple algorithms or for exploring work in the field of Active Learning, that we leave as future work.

5.4 Data Preparation

The *Extraction-Transformation-Load* (ETL) procedure summarized with the Apache Spark block in figure 5.2 incorporates multiple steps and it includes important design decisions heavily dependent on the specific algorithms that we use in the Data Analytics core presented in the Chapter 6. Before starting with a careful description of every step we summarize in Table 5.1 all the temporal scales of the analysis chosen in Section 2.6. In Table 5.2 we summarize instead the names of the metrics used together with the *Collectd* plugin that is responsible for their production.

5.4.1 Discretization of Time Series

The rate at which every metric is produced by an hypervisor and goes into the monitoring infrastructure is unpredictable because of network or processing delays. In addition, different configurations for different sensors are

Variable	**Description**	**Chosen Value**
w	Window Length	48 (nr timesteps)
x	Temporal Length of one timestep summarized in a single data point.	10 (minutes)
m	Number of metrics used in a window of analysis.	11 (metrics)

Table 5.1: Temporal Scales of Analysis. We refer to the same nomenclature of Section 2.6

Collectd Plugin	**Metric's name**
CPU	cpu_percent_idle
CPU	cpu_percent_system
CPU	cpu_percent_user
Interface	interface__if_octets__tx
Interface	interface__if_octets__rx
Load	load_longterm
Memory	memory__memory_free
Swap	swap_swapfile_swap_free
Swap	swap_swapfile_swap_used
VMEM	vmem__vmpage_io_memory_in
VMEM	vmem__vmpage_io_memory_out

Table 5.2: Selected Metrics and their Collectd plugin of origin.

directly responsible for different production rate of the relative timeseries. Therefore in these cases we have an unbalanced situation with many more readings for a sensor with respect to the others. As mentioned in our modelling part (Section 2.5), we decide to convert every time series in a *Discretized Time Series* (Definition 2.5.1). In practice we aggregate our data per machine and per sensor in non overlapping intervals of 10 minutes and we keep the statistical mean of the sensor's reading in that temporal range as summary. The implementation has been done in a distributed way using the Spark DataFrame API and is available in the Appendix C.3.2.

5.4.2 Input Normalization

The metrics collected by the hypervisor's sensors carry specific information such as memory available, CPU usage, disk operations, network activity. Each of them represent a different quantity that might be a percentage, a real or discrete value, and most importantly they have typically many order of magnitudes of difference, for example *CPU load* represents a percentage (between 0 and 100) whereas *SWAP space free* is in the order of Gigabytes, namely 10^9. This difference in scale of the various metrics is harmful for some anomaly detection algorithms since they will erroneously weight more the metrics with higher value, in particular those that use distance measures like LOF and KNN. We therefore normalize the data based on our training set and separately for every metrics. In particular we standardize by removing the mean and dividing by the standard deviation:

$$x_{normalized} = \frac{x - \mu_m}{\sqrt{\sigma_m}} \tag{5.1}$$

where m is an hypervisor metric and μ_m, σ_m are respectively mean and standard deviation of that metric computed on the training set (one week of data) and considering all the hypervisors together. The implementation of this step is available in the Appendix C.3.3.

5.4.3 Minimal Unit of Analysis

Every algorithm is design to take as input a single Multivariate Temporal Window (Definition 2.5.3) at a time and produce an anomaly score; this window refers to a specific hypervisor and a specific time interval covered by the window itself. Given the differences between traditional Machine Learning method and Deep Learning ones, we adapt the input based on the methods. In particular, the vast majority of the traditional methods (Section 3.3) are not able to model the temporal dimensional, therefore we propose two distinct input data formats:

- *greymap* representation: that corresponds to the matrix representation described in Definition 2.5.3. Here the temporal dimension is preserved in one axis of the matrix.
- *vectorized* representation: where all the different metrics and their timesteps present in the window are flattened and each timestamp of each metrics becomes a simple feature of our datapoint.

In particular we use the *greymap* representation for algorithms that can model the temporal dimension (AECNN, AELSTM, FORVAR, FORCNN) and the *vectorized* representation for those not able to model it (OCSVM, LOF, KNN, PCA, IFOR and AEFC). We also refer to methods taking the *vectorized* representation as *static* anomaly detection methods because they are suitable for all kind of dataset with features without taking into account in any way the temporal information.

In both cases the input contains the same amount of data, it consists in a temporal window of data containing w time steps in the past and m time series related to the same same hypervisor. The window length is $w = 48$ where every time step summarizes 10 minutes of data with the mean. In total every window represents the last 8 hours of metrics for a specific hypervisor as described in the Problem Formulation with the concept of Multivariate Temporal Window (Definition 2.5.3).

5.4.4 Greymap for TimeSeries AD Algorithms

The *greymap* representation corresponds to what we think as the most natural representation of a time window, that is the matrix representation described in our Problem Formulation as Multivariate Temporal Window (Definition 2.5.3). Each row contains the values of a single metric in that window of time and therefore the columns refers to subsequent timesteps of the sensors' values. We report here the version given by the Definition 2.5.1 declined with the specific number of metrics (m=11) and timestamps ($w = 48$) we are considering in our pipeline:

$$greymap_i = \begin{pmatrix} d_i^1 & d_{i+1}^1 & \cdots & d_{i+47}^1 \\ d_i^2 & d_{i+1}^2 & \cdots & d_{i+47}^2 \\ \vdots & \vdots & \ddots & \vdots \\ d_i^{11} & d_{i+1}^{11} & \cdots & d_{i+47}^{11} \end{pmatrix} \tag{5.2}$$

The name *greymap* comes from the visual representation we adopt to inspect data with a heatmap plot (Figure 5.3).

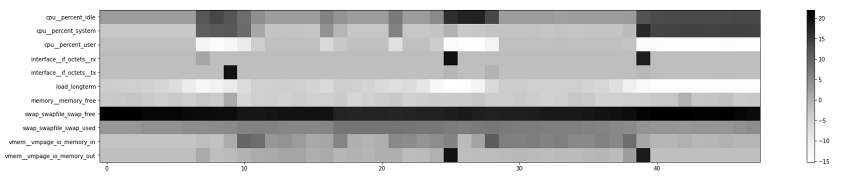


Figure 5.3: Greymap representation. It consists in a heatmap that represents the timeseries input for a single hypervisor, each row is the timeseries of one of the many timeseries M metrics considered in this multivariate setting (in this case, M = 11). Each column represent the past timesteps in a window of length w (in this case, w = 48).

5.4.5 Vectorization for Static AD Algorithms

In alternative, for methods that are used to one dimensional input we have to discard the temporal information and condense all the data from different metrics (i.e. rows) in a single vector. We call this procedure *vectorization* and the resulting encoding a *vectorized* encoding of our window. By applying this process, we accept to lose some information since we do not have anymore a direct representation of time in this representation. The final formalization of this vector is the following:

$$vectorized_i = [d_i^1, d_{i+1}^1, \cdots, d_{i+47}^1, \cdots, d_i^{11}, d_{i+1}^{11}, \cdots, d_{i+47}^{11}] \qquad (5.3)$$

5.5 Production Implementation with Apache Airflow

We adopt Apache Airflow [1] as the main orchestrator for all the steps of our pipeline. It is an open-source workflow management platform initiated by Airbnb in October 2014, where a workflow can be defined asa Directed Acyclic Graphs (DAGs). Each node of the DAG represents a step in the piplene and is implemented with an *Airflow operator* [2]. In Figure 5.4 we see our implementation and the Bash Operator node used to schedule bash commands. Moreover Airflow can handle also repetitive analysis scenarios, where a predefined number of tasks has to be repeated every fixed amount of time. In particular for our experimental part we repeated the analysis every week, visible in Figure 5.5. The steps encoded are the following:

1. prepare the configuration file containing the information about which group of hypervisors we want to monitor, metrics we want to consider and interval for our training set and testing set;

2. download the training data and normalize them by computing and storing the normalization coefficients for every metric;

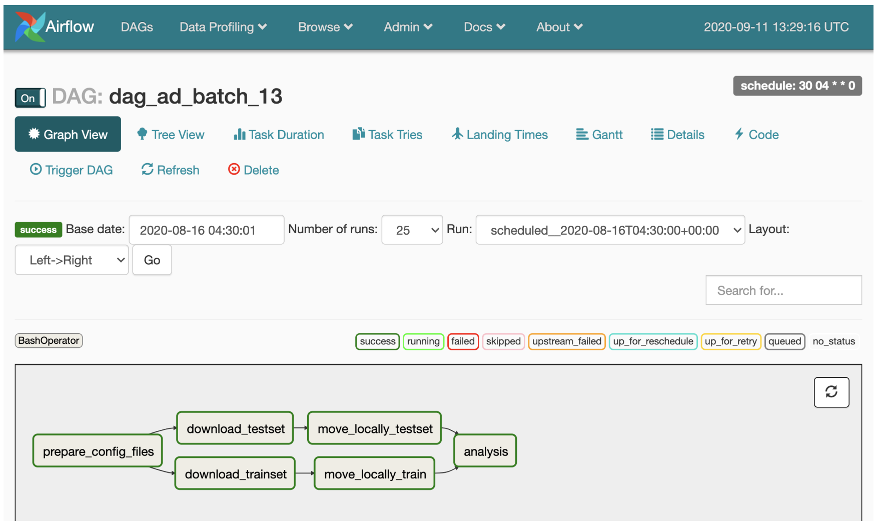
3. download the testing data and normalize them with the normalization computed on the trainset;

4. run the analysis on the downloaded data, with train on the trainset and test on the testset;

[1]Apache Airflow Project Description: `https://airflow.apache.org/docs/stable/project.html`

[2]Airflow Operators: `https://airflow.apache.org/docs/stable/_api/airflow/operators/index.html`

Note that every step, apart from the configuration files' preparation is run in a Docker container environment to have a precise definition of the libraries necessary in every step. In addition the last step has two possible optional outputs for the anomaly score, they can either go to the real monitoring infrastructure via a Fluentd [3] logging driver attached to the container or either be saved in a local file for benchmark production.



Base date: 2020-08-16 04:30:01 Number of runs: 25 Run: scheduled__2020-08-16T04:30:00+00:00 Layout: Left->Right

Figure 5.4: Airflow Production DAG. Direct Acyclic Graph representing the task done for analysing one week on data with the various algorithms. Note that the step of data preparation is split in two sub steps (download_*, move$_l$*ocally_∗), becausetheaggregationhappensonlyinApacheSparkgiventhelargevolumeofdataprocessedand

[3]Fluentd is an open-source data collector for unified logging layer. More info can be found here: https://docs.fluentd.org/

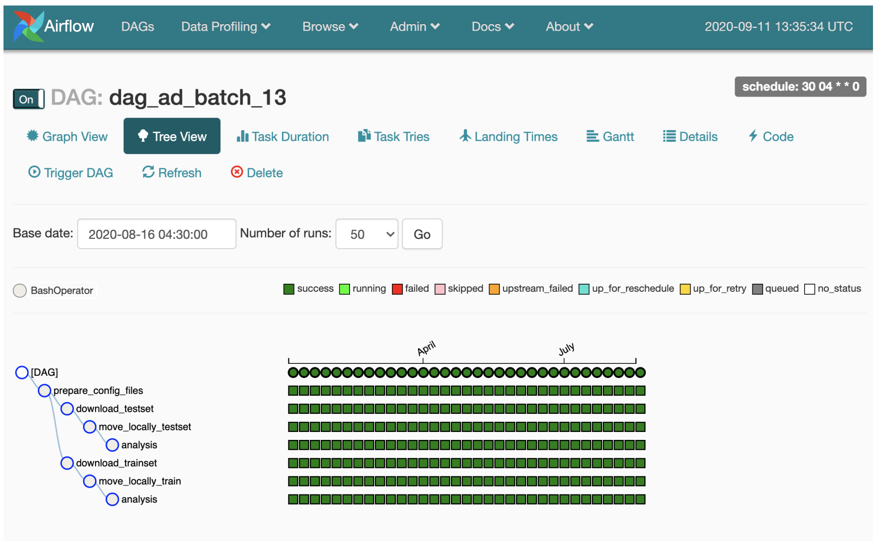


Figure 5.5: Airflow Recurrent Analysis. Recurrent analysis happening for every week of data in a Batch group of hypervisors.

Chapter 6

Anomaly Detection Solution: Data Analytics Core

The main component of the system described in Chapter 5 is the Data Analytics core that contains the actual algorithms and methods to discover anomalies. We select both Anomaly Detection methods related to traditional Machine Learning (ML) and Deep Learning (DL). For each of those category we also propose one method that is specific for time series. They are summarized in Table 6.1 and they are divided in the two families.

Traditional ML	**Deep Learning Based**
One Class SVM (OCSVM)	AutoEncoder Fully Connected (AEFC)
Local Outlier Factor (LOF)	AutoEncoder with CNN (AECNN)
Isolation Forest (IFOR)	AutoEncoder with LSTM (AELSTM)
Principal Component Analysis (PCA)	Forecaster based on CNN (FORCNN) - *Time Series Specific*
K-Nearest Neighbors (KNN)	
Forecaster based on Vector Autoregression (FORVAR) - *Time Series Specific*	

Table 6.1: Summary of methods under study divided in the two main categories: Machine Learning and Deep Learning. In addition the last line refers to methods specific for Time Series Anomaly Detection.

The idea of including traditional Machine Learning methods is also motivated by the presence of a vast amount of literature in the Outlier Detection methods for non temporal data. Testing their performance and suitability for the CERN use case is crucial to justify the usage of more powerful but computational intensive methods. For the implementation point of view, since CERN requires solid software tools for a production environment we select the reliable and well tested PyOD library [1] that is also attracting interest of both industry and academia [52].

6.1 Train Set and Test Set

For our training and test dataset we decided to work on weeks of data with our choices summarized in the Table 6.2, with one week for train and one week for test. This procedure is then repeated for every couple of consecutive weeks of the two curated CERN datasets. During train we fit our models with data in an unsupervised way. Deep Autoencoder models learn their reconstruction objective: AEFC, AECNN, AELSTM. Forecasting methods fit the data to get a low prediction error. PCA learns the projection, KNN and LOF keep the samples in memory for comparison at test time. Moreover we also store the mean and standard deviation of every input metric data, that we then use to normalize all the training data of the train week. We also save the mean and standard deviation of the anomaly scores computed on the train week.
At test time we normalize the metrics data of the test week with the mean and standard deviation of the week of train, so that the metrics are in a similar range, then we apply the algorithms and get an anomaly score for every windows in the test week.

6.2 Normalization Anomaly Score

An important design choice common to all algorithms is the Anomaly score normalization. We normalize the test anomaly scores with the mean and standard deviation of scores obtained on the train week. Here we assume that this statistical quantities remain quite stable from a week to the next one, in particular for the normal instances. We do this step to guarantee that all the methods get more or less the same range of anomaly scores and the comparison between them is in the same scale. This is also beneficial for the ensemble strategies that will combine similar quantities.

[1]Python Outlier Detection https://github.com/yzhao062/pyod

Variable	**Description**	**Chosen Value**
$tmp(X_{train})$	Temporal length of covered by the training dataset.	1 (week from Sunday at 00:00 to Saturday at 23.59)
$tmp(X_{test})$	Temporal length of covered by the testing dataset. Note that the time of testing is always directly temporally contiguous to the training dataset.	1 (week from Sunday at 00:00 to Saturday at 23.59)

Table 6.2: Temporal Scales of Analysis. We refer to the same nomenclature of the Problem Formulation

6.3 Novel Time Series Methods

Beside the adaptation of traditional outlier detection methods we propose also adaptation of forecasting methods introduced in the Section 3.5.1 to our Problem Formulation. They are usually performant in detecting *point anomalies*, namely when a single point is anomalous in the entire time series. Nonetheless in our formulation we are aiming at labeling regions (i.e. windows) of the time series that are showing an unexpected behavior. Therefore we adapt them by aggregating the anomaly score for each point in the window in a single anomaly score using the summation of prediction errors on different time steps:

$$s_{forecast}(W_{m,w}) = \sum_{i=1}^{w} \sum_{j=1}^{m} (d_i^j - \hat{d}_i^j)^2 \tag{6.1}$$

where i is the temporal index among the w timesteps of the window $W_{m,w}$, j refers to the m metrics of our multivariate scenario and $\hat{d}_i^j$ is the prediction of the model produced from the historical data preceding the i^{th} timestamp.

6.3.1 Forecasting with VAR

Among the traditional Time Series models introduced in 3.5.2, we choose to use the Vector Autoregressive (VAR) model for our CERN use case, since it works on multi-time series scenario and the prediction of a metric's value can be dependent on the past values of other metrics too. One limitation of the VAR model is that it can only learn from complete timeseries belonging to the same hypervisor. It is not trivial to decide how to learn parameters from windows belonging to different hypervisors. Our solution consists in creating an ensemble of models, each of them learned on a different single hypervisor and to contain the computational cost we learn only on a random subset of the hypervisors in the group. Then at test time we use those single model together to asses the abnormality of all the hypervisors in the groups, even those for which we did not learn a specific model. In this way we assume that the selected subset of machine is a good representation of the normal behaviour and we expect it to generalize well also on new unseen hypervisors.

The order of a single model is set once and for all the models in the ensemble to $p = 2$ by minimizing the Akaike information criterion (AIC), that is a measure of quality of a predictor that rewards the goodness of fit but considers also the complexity of the model in term of number of parameters to estimate. This is the formula:

$$AIC = 2k - 2ln(L) \tag{6.2}$$

where k is the number of parameters and $\hat{(L)}$ is the likelihood of the model on the data.

Given an ensemble model composed of $c = 20$ individual models learned on the same number of hypervisor, we have two levels of aggregation for the creation of the anomaly score:

- **window-level**: each single VAR model is given 2 timesteps of history in our window and predicts the next timestep. Then we compute the euclidean distance between prediction and the actual data to find an error measure. Since our window is $W = 48$ timesteps long we repeat this for 46 times. The first aggregation level consists in summing all the errors of the various timestep to create an overall anomaly score for this window.

- **models-level**: the presence of $c = 20$ models will give us c different window-level anomaly score that we aggregate them taking the mean

The overall formula is the following:

$$s_{VAR}(W_{m,w}) = \frac{1}{c}\sum_{i=1}^{c}\sum_{j=p}^{w}(VAR\_model_i(W_{m,w}(j-p,j)) - W_{m,w}(j))^2 \tag{6.3}$$

where c is the number of models in the ensemble, p the order of the VAR model, $VAR\_model(\cdot)$ is the prediction of one model, $W_{m,w}(a, b)$ is the Multivariate Temporal Window matrix (Definition 2.5.3) from column in position a to position b excluded and $W_{m,w}(a)$ is just the column at position a of that windows.

6.3.2 Forecasting with CNN

We employed a model inspired by LeNet [53], with few layer of CNN followed by a funnel of densely connected layer. In a given window with W timesteps and m time series we represented it as an image, that we defined *greymap* in Section 5.4.4.

The convolution operation has a certain receptive field of dimension $3 \cdot m$, so that every convolution operation can take information from all the other m timeseries as well from the neighbouring timesteps.

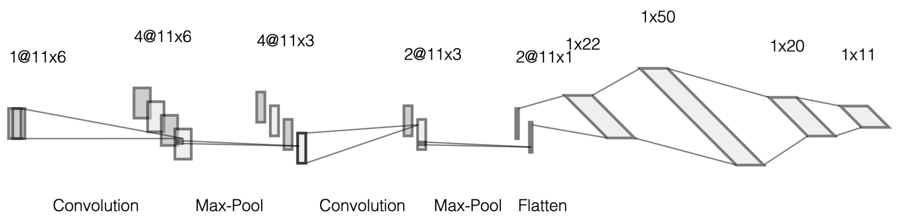


Figure 6.1: CNN Forecaster architecture

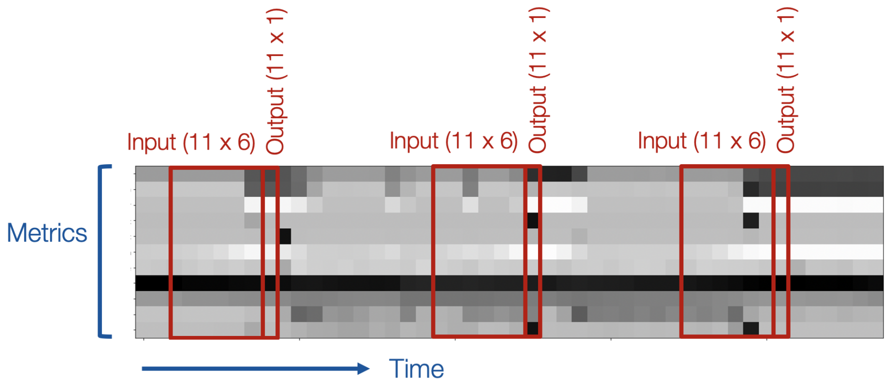
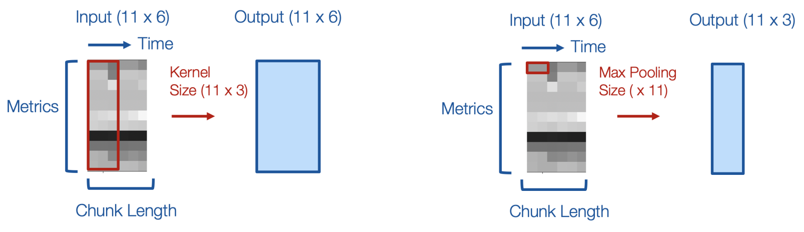


Figure 6.2: Sliding predictions that can be done on a single greymap. Here we show 3 of the total 42 *pairs of Input-Output squares that are used to produce the reconstruction error.*

Online Anomaly Detection method focused on point anomalies would use the entire window of $w - 1$ timesteps to forecast the current timestep with the CNN model, but since we are interested in anomalies appearing in the entire window we adopted a different approach. Instead we trained the Neural Network model by feeding a shorter segment of the image with H consecutive timesteps (where $H < w$) and then predict the next timestep after the shorter chunk of length H. The model prediction is then compared with the real value to compute the prediction error. Then an overall anomaly score is created by summing all the prediction errors in the window. We are intuitively applying the same approach used for point anomalies but replicated for every timestep of the window. A typical example where we have $w = 48$ a reasonable value could be $H = 6$.



(a) Convolutional Operation (b) Max-Pooling

Figure 6.3: Details about the convolutional and max-pooling operations used in the proposed network.

6.4 Autoencoders for Time Series Modelling

As described in the Background 3.4.1 the most popular Deep Learning architecture is the Autoencoder, therefore, taking inspiration from previous literature [29, 30, 32, 35], we propose our simple versions of those Autoencoder variants.

6.4.1 Fully Connected Autoencoder

We propose a fully connected neural network architecture with 1 input layer to take our *vectorized* representation as input, 3 hidden layers to implement the bottleneck principle and 1 output layer to produce another vector with the same dimension of the input. A indicative representation is given in Figure 6.4 We adapt the PyOD implementation of this method to work with the latest version of TensorFlow 2.1.

6.4.2 CNN Autoencoder

We propose an architecture made of an alternation of convolution and max pooling operations for the encoder part and convolution and up-sampling for the symmetric decoder side. As anticipated, the input of this method

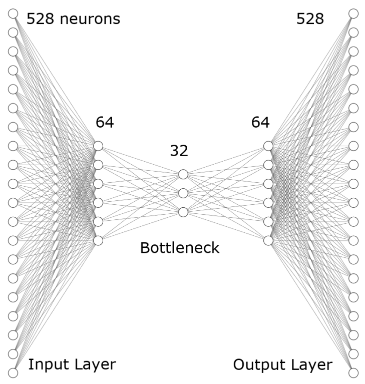


Figure 6.4: Fully Connected Autoencoder architecture. It is made of five dense layer of 528, 64, 32, 64, 528 neurons respectively. Note that the number of neurons is just smaller to avoid cluttering the diagrams with edges.

is the *greymap* representation that serves as an image in our case, but contrary to usual kernels used for traditional image processing we designed our convolutional kernel to dimensions able to cover all the metrics when sliding in the temporal dimension. Moreover, for the input reduction with max pooling operation we reduce the dimension of the area span by it so that it summarizes with the max only pixel from the same metrics. We keep avoid to put more layers to keep the training relatively fast. Figure 6.5 shows the details of the architecture.

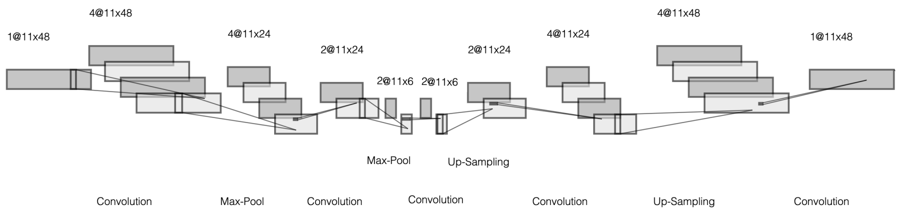


Figure 6.5: CNN Autoencoder architecture

6.4.3 LSTM Autoencoder

We design an architecture made of two LSTM layers that with hidden state of dimension 10. We keep this representation relatively low to ease the train and also because we want to enforce the bottleneck principle in this way. Figure 6.6 shows the overall architecture and also the hidden states movement.

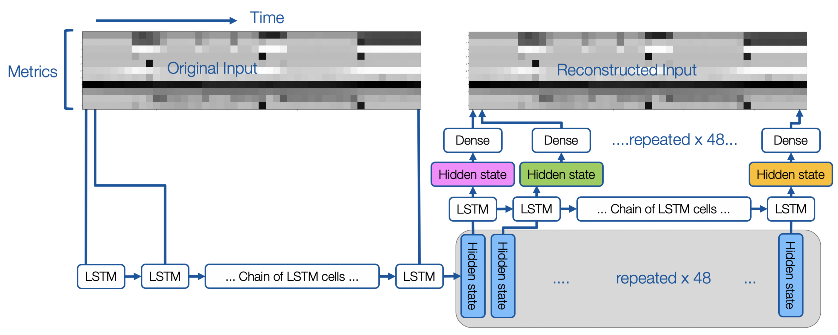


Figure 6.6: LSTM Autoencoder architecture. Note that the blue hidden state is just the last hidden state of the pass in the first layer and it is repeated to match the number of timesteps (48), whereas the second LSTM layer is producing different hidden layers and from each of them we produce a timestamp in the output image (that corresponds to a column). Note that the reconstructed image shown as output is the ideal situation and it has not been produced by our algorithm in the real use case.

6.5 Ensemble

Thanks to the normalization of anomaly scores explained in Section 6.2 we explore the way to combine the prediction produced by different models. Indeed this normalization steps corresponds to the one described by [41] and introduced in Section 3.6.1; it converts all the anomaly scores in the same intervals so that they are comparable in size. We explore some of the aggregation techniques introduced in the Section 3.6.1: max, min, median, average.

6.5.1 Linear Regression Ensemble

In addition we propose a novel combination technique that makes use of some annotated labels. We call it *Linear Combination* and consists in fitting a linear regression classifier that combines the scores form different methods learning a linear combination of them based on some labels:

$$\textit{ENS-LINREG}(W_{m,w}) = \sum_{m \in \text{Methods}} c_m \cdot s_m(W_{m,w}) \tag{6.4}$$

where c_m is the weight learned by the Linear Regression and assigned to method m, whereas $s_m(W_{m,w}$ is the anomaly score assigned by method m to the window $W_{m,w}$. In particular it can be sees as higher level learning procedure since we learn how to combine predictions made by other learners.

Note that we use 10 days of the two curated datasets of *Batch* and *Shared* hypervisors learn the regression coefficients and then we remove those windows of data from the computation of the performance metrics.

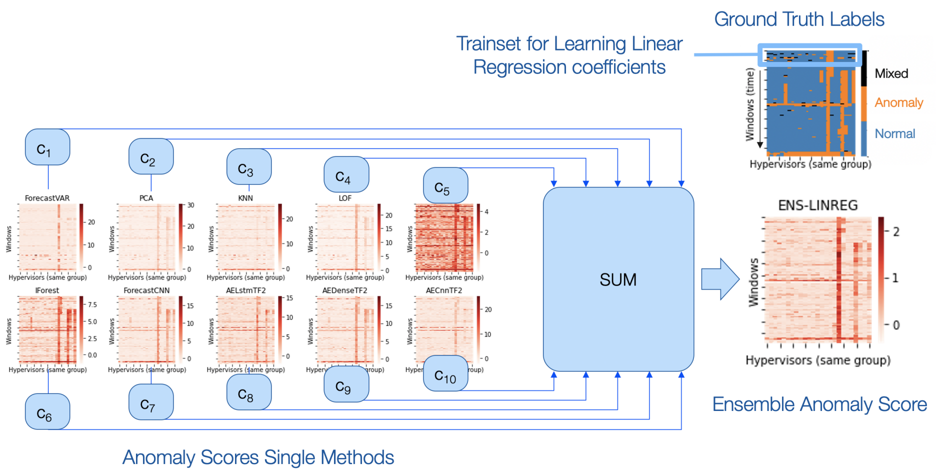


Figure 6.7: Linear Regression Ensemble. We can see the various anomaly score prediction matrix of the single algorithms on the Batch case. Every matrix represent the anomaly scores of the single hypervisors, corresponding to columns, through time, represented by the vertical axis. The linear regression coefficients are learnt form the first days of the ground truth labels.

Chapter 7

Experimental Settings

Given the interest in the CERN use case the focus is on assessing the performance on CERN data. We identify two scenarios:

1. **Experiment A: Two Curated Annotated Dataset from CERN**: collected thanks to the new functionalities and user interface introduced with our extension to the Grafana CERN monitoring dashboard. They are collected by CERN domain experts on one *Batch* Openstack Cell and one *Shared* Openstack Cell as described in Chapter 4.

2. **Experiment B: Artificial Anomalies**: following the directives of [51] we combine time series coming to two different real world process representing the two user categories introduced in the Problem Formulation. The *Batch* time series are considered normal data, while the more irregular and diverse *Shared* time series are considered anomalous. For details refer to the description given to 4.5.

Another option present in the literature [47] is the *Server Machine Dataset (SMD)*, but it is not compliant with our problem formulation since it has been designed for point anomaly detection.

7.1 Figure of Merits

Every method under study produces an anomaly score, therefore by applying a threshold as explained in 2.4 is evaluated with the same performance metrics of a binary classifier, where the positive class is represented by label 1 and corresponds to an anomalous instance, whereas the negative one corresponds to label 0 and means normal instance. We therefore define the following four quantities:

- True Positives (TP) or True Alarms: number of anomalous hypervisors that the algorithm correctly identifies as anomalies.
- True Negatives (TN): number of healthy hypervisors that the algorithm correctly identifies as normal.
- False Positives (FP) or False Alarms: number of healthy hypervisors that the algorithm *wrongly* identifies as anomalies.
- False Negatives (TN): number of anomalous hypervisors that the algorithm *wrongly* identifies as normal.

Those four situations are summarized in the Figure 7.1, then with those we build the derived metrics described in the sub sections that come next and summarized in the table.

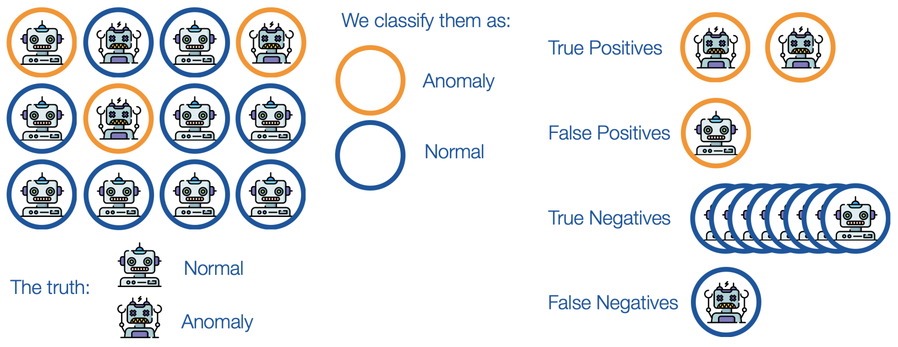


Figure 7.1: Main metrics to evaluate a binary classifier. On the left we see a group of machines represented by robot icons, it can be either normal or anomalous. Then the binary classifies can declare it as normal (blue circle) or anomalous (orange circle). On the right we have the four possible situations where the algorithms is good at spotting anomalies (True Positives) or normal data (True Negative) and where it is bad, spotting false anomalies (False Positive) or false normal data (False Negative).

7.1.1 Receiver Operating Characteristic

In this alarming context the most relevant metrics for assessing the performance of an Anomaly Detection method is the False Positive rate since the expert do not have enough time to cope with many False Alarms given the limited amount of time. Comparing also to similar literature [54], the Receiver Operating Characteristic (ROC) is the tool used to compare the methods under study in terms of True Positive Rate (TPR) and False Positive Rate (FPR). The ROC consists in plotting the TPR on the y-axis and the FPR on the x-axis for different values of thresholds for the anomaly scores to discern between normal and anomalous. They are computed with the following formulas, where P and N are respectively the total number of anomalies and normal data:

$$TPR = \frac{TP}{TP + FN} = \frac{TP}{P} \tag{7.1}$$

$$FPR = \frac{FP}{FP + TN} = \frac{FP}{N} \tag{7.2}$$

The main reason for using it in this context is that we do not have to choose a threshold for every algorithm but we can compare their performance with various threshold values. In addition we also use the Area Under the Curve (AUC-ROC) to summarize the performance of the algorithms in a single number. It consists in the integral of that curve and therefore the possible values ar in the range $(0, 1)$ with 1 being the best. Even though some limitations have been reported for specific contexts [55], we still believe it is a good indicator to consider together with other metrics.

7.1.2 Precision, Recall, F1 Score

Other indicators we import from the Information Retrieval literature are the following:

$$Precision = \frac{TP}{TP + FP} = \frac{\text{Nr Good Prediction of Anmalous Hypervisors}}{\text{Nr Hypervisors Predicted as Anomaly}} \tag{7.3}$$

$$Recall = \frac{TP}{TP + FN} = \frac{\text{Nr Good Prediction of Anmalous Hypervisors}}{\text{Nr of real Anmalous Hypervisors}} \tag{7.4}$$

$$F1 = \frac{2 \cdot \text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}} \tag{7.5}$$

We highlight that the Recall coincides with the True Positive Rate used in the ROC and the F1 score is the harmonic mean of the other two indicators: Precision and Recall.

7.1.3 Distribution of Anomaly Score

The final goal of the anomaly score is to discern between normal instances and anomalous ones. Therefore the distribution of anomaly score of the two groups is crucial to visually verify that the two distributions can be separated with a threshold on the anomaly score value. In fact, in a good algorithm for Anomaly Detection we expect that the normal instances are have mostly a lower score than the anomalous ones, which on the contrary should have a higher anomaly score.

7.1.4 Average Training Time

Beside the detector performance's metrics, training time is another crucial characteristic to compare methods used in an operational context such as the one at CERN.

7.1.5 Similarities among Methods

Once we have single methods' results then we want also to see if they are significantly different from each other. Kendall's Tau coefficient [44] is an option proposed by [56] to measure the accordance between two anomaly detection rankings (Section 3.6.1) in view an increased diversity required for the creation of a good ensemble strategy. We considered the original formulation of [44] and the implementation of scipy [1]:

$$\tau(a,b) = \frac{(P-Q)}{\sqrt{(P+Q+T)\cdot(P+Q+U)}}$$

where a and b are the two rankings and P is the number of concordant pairs, Q the number of discordant pairs, T the number of ties only in a, and U the number of ties only in b. Note that ties that are present in both rankings are not considered.
Nonetheless the ranking approach has a very important limitations that is present if applied to our scenario. In fact the longer the rankings compared are the more probable it is to have a low coefficient, and consequently low measured similarity. Therefore we confine the use of Kendall's tau only to analysis of a single week of data, whereas for the comparison of all anomaly score we rely on the correlation of normalized anomalies scores. In fact after the normalization of the anomaly scores, we have that every algorithm assigns a score that is somehow centered in zero on training data, therefore we can compare their similarities from a scatter plot represented each window of data analysed with the x and y coordinate corresponding to the normalized score of the two algorithms.

[1]Scipy Python library: `https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.kendalltau.html`

7.2 Experiment A - CERN curated Dataset

We run the analysis of the data on about six months of annotated data. We repeat this experiment for both a **Batch** and a **Shared** group separately. We analyse the non-overlapping window data with the selected algorithms. Therefore for each method we produce the anomalies scores of every hypervisor in the two Openstack cells under study for a length of around six months. In a final step we compare the produced anomalies scores with the ground truth labels collected by our experts and produce the ROC curve and compute the AUC, Precision, Recall, False Positive Rate and F1. Note that not all the data are completely annotated, therefore we exclude the windows for which a hypervisor is not annotated from the computation of these performance metrics. These are the performance metrics on the two cases:

- *Batch* dataset (described in Section 4.4.1). Complete results are visible in the Appendix in Figures B.1 and B.2 for Traditional and Deep methods respectively.

- *Shared* dataset (described in Section 4.4.2). Complete results are visible in the Appendix in Figures B.3 and B.4 for Traditional and Deep methods respectively.

7.2.1 Formalized Train and Test Procedure

For the comparative study, we adapt the all the methods to work with the same quantity of input data both at train and test time, the only difference is in the format, either *greymap* of *vectorized.* In the Algorithm 1 we summarize the steps we undergo both during training and test for a single algorithm. The main points concern the fact we train on one week and test on the consecutive week, and we rank one window of data at a time. Moreover, we have a two step normalization procedure as explained in Sections 5.4.2 and 6.2, we normalize the data to have the features in the same range and we normalize the anomaly scores to have the various methods producing a score centered in zero for the normal case. Note that in the Train procedure (Algorithm 2) we create all possible windows form the train data, we also allow overlapping windows, therefore for example with $x = 10$ minutes, that means that a datapoint summarizes 10 minutes of data, and $w = 8$ hours we have 144 different windows for every hypervisor in one day. On the other hand for the Test procedure (Algorithm 3) we create only non-overlapping windows that can be created within the current week test data, with the same parametrization just mentioned we will have 3 different windows for every hypervisor in one day. Another note on the amount of training data, for the Deep learning one that are data greedy we give all the possible windows as input, whereas for the traditional method we subsample 1000 samples since they are not scaling as well as the Deep methods, especially those parametric like KNN and LOF that store the data seen at train time.

Algorithm 1 Train-Test Procedure

```
1: all_results = empty list                              ▷ Prepare the result list
2: dataset = either Batch or Shared Dataset         ▷ Select your benchmark Dataset
3: weeks = split(dataset) ▷ Divide my dataset in chunks of one week each
4: sorted_weeks = sort(weeks)                     ▷ Sort the weeks, the oldest first
5: algo = initialize algorithm
6: for index in range[1, len(sorted_weeks)] do              ▷ Iterate over weeks
7:     current_week = sorted_weeks[index]
8:     previous_week = sorted_weeks[index - 1]
9:     (tr_data_means, tr_data_st_devs, tr_mean_score, tr_st_dev_score) = TRAIN(previous_week, algo)
10:    week_results = TEST(current_week, algo, tr_data_means, tr_data_st_devs, tr_mean_score, tr_st_dev_score)
11:    all_results.append(week_results)
12: end for
```

7.2.2 Algorithms Training Time

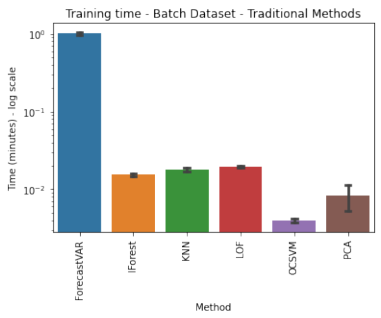
In Figure 7.2 and 7.3 we summarize the training time respectively for the traditional and deep methods, we recall that every algorithm undergoes an entire training procedure for every week. An important decision that heavily influence the comparison between deep and traditional methods consists in not feeding to the traditional algorithms only a subsample of size 1000 windows among all the possible windows we can build with the week of training data.

Algorithm 2 Train Routine

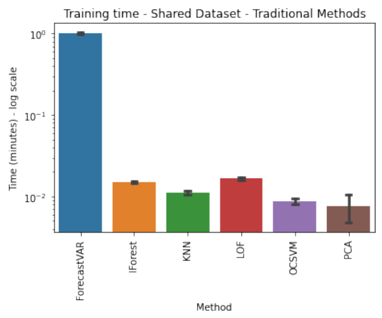
```
1: procedure TRAIN(previous_week, algo)
2:     previous_week = sorted_weeks[index - 1]
3:     tr_means = empty list                         ▷ Vector of metrics' means
4:     tr_st_devs = empty list                       ▷ Vector of metrics' st.dev.
5:     for m in metrics do
6:         mean_m, st_dev_m = get_mean_stdev(previous_week, m)
7:         tr_means.append(mean_m)
8:         tr_st_devs.append(st_dev_m)
9:     end for
10:    std_prev_week = standardize(previous_week, tr_means, tr_st_devs)
11:    train_dataset = get_all_possible_windows(std_prev_week)
12:    if algo is not Deep Learning then
13:        train_dataset = subsample(train_dataset, n=1000)
14:    end if
15:    algo.fit(train_dataset)                        ▷ Train the algorithm
16:    train_anomaly_scores = algo.assign_score(train_dataset)
17:    tr_mean_score = mean(train_anomaly_scores)
18:    tr_st_dev_score = st_dev(train_anomaly_scores)
19:    return (tr_means, tr_st_devs, tr_mean_score, tr_st_dev_score)
20: end procedure
```

Algorithm 3 Test Routine

```
1: procedure TEST(current_week, algo, tr_means, tr_st_devs,
   tr_mean_score, tr_st_dev_score)
2:     week_results = empty list
3:     st_current_week = standardize(current_week, tr_means, tr_st_devs)
4:     test_dataset = get_non_overlapping_windows(std_current_week)
5:     test_anomaly_scores = empty list
6:     for window in test_dataset do
7:         w_score = algo.assign_score(window)
8:         n_w_score = normalize(w_score, tr_mean_score, tr_st_dev_score)
9:         week_results.append(n_window_score)     ▷ Add also information
   about hypervisor and time of end of the window
10:    end for
11:    return week_results
12: end procedure
```

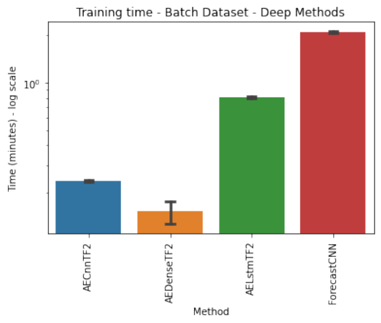


(a) Run on the *Batch* dataset.

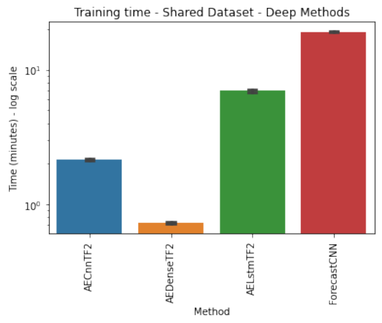


(b) Run on the *Shared* dataset.

Figure 7.2: Training Time of Traditional methods under study. We see the mean value and variance (error bar) of the time required by the specific method to train on one week of data. They are trained only on a random subsample of 1000 *windows, to avoid scale issue on parametric methods. Note that the y-axis is in log-scale.*



(a) Run on the *Batch* dataset.



(b) Run on the *Shared* dataset.

Figure 7.3: Training Time of Deep methods under study. We see the mean value and variance (error bar) of the time required by the specific method to train on one week of data. The number of epochs of train is 20. Note that the y-axis is in log-scale.

7.2.3 Area Under Curve - ROC

In Table 7.1 and 7.2 we report all the mean and variance of the Area Under the Receiving Operating Characteristic Curve (AUC-ROC) for all methods: traditional, deep and ensemble. The mean and variance are computed along the various runs, one per week, for a total of 26 runs in the *Batch* case and 32 for the *Shared* one.

Method	Mean	StD
KNN	0.697	0.173
LOF	0.877	0.168
PCA	0.910	0.124
OCSVM	0.814	0.140
IForest*	0.921	0.134
ForecastVAR	0.704	0.234
AEDenseTF2	0.909	0.124
AECnnTF2	0.753	0.208
AELstmTF2	0.829	0.203
ForecastCNN	0.910	0.159
ENS-MAX	0.883	0.158
ENS-MIN	0.739	0.196
ENS-MEDIAN	0.884	0.153
ENS-AVERAGE	0.877	0.158
ENS-CUMSUM	0.877	0.158
ENS-LINREG	0.833	0.218

*Table 7.1: AUC-ROC all methods on Batch. It is computed as average on all the weeks for the Batch scenario. The best mean is highlighted with a *.*

Method	Mean	StD
KNN	0.739	0.065
LOF	0.698	0.121
PCA	0.713	0.137
OCSVM	0.693	0.084
IForest	0.752	0.092
ForecastVAR	0.724	0.095
AEDenseTF2	0.713	0.139
AECnnTF2	0.777	0.071
AELstmTF2*	0.793	0.058
ForecastCNN	0.715	0.138
ENS-MAX	0.754	0.092
ENS-MIN	0.717	0.087
ENS-MEDIAN	0.750	0.103
ENS-AVERAGE	0.768	0.096
ENS-CUMSUM	0.768	0.096
ENS-LINREG	0.774	0.122

*Table 7.2: AUC-ROC all methods on Shared. It is computed as average on all the weeks for the Shared scenario. The best mean is highlighted with a *.*

7.3 Experiment B - CERN Artificial Setting

As described in Section 4.5, in this artificial setting we merge *Batch* and *Shared* considering them respectively normal and anomalous data. In practice, We start from a week of windows of 183 *Batch* hypervisors and a week of 200 *Shared* hypervisors, we divide them into windows of 8 hours. Subsequently we iterate over all the non overlapping 8 hours intervals of *Batch* windows and we train every method on the 183 *Batch* hypervisors then we test its performance by scoring the same 183 *Batch* hypervisors plus 91 *Shared* hypervisors extracted form the week of *Shared* windows. The quantity of injected windows is chosen to keep 2:1 relationship between normal and anomalous data.

In the ideal case the methods should be able to tell if at test time an hypervisor is a *Batch* or *Shared* one assigning respectively a low and high anomaly score. To increase the difficulty of the artificial task we select the *Shared* hypervisors to inject based on a similarity score with the *Batch* hypervisors in the same window. The similarity score is computed with the dot product of the normalized vectors representing the hypervisors, we select the one that is on average most similar. Moreover we design three different scenarios of increasing complexity:

- **unprocessed data**. We keep the data unprocessed, they have their original mean and variance, and the disproportion among metrics is also left untouched, meaning that for example the *CPU idle* is a percentage while the *SWAP space free* is a number in Gigabytes therefore billions.
- **same mean**. We report both windows form *Shared* and *Batch* hypervisor to have zero mean on all the input metrics.
- **same mean and variance**. We report both windows form *Shared* and *Batch* hypervisor to have zero mean and unit variance on all the input metrics.

Given that the performance of the final anomaly detection system is not measured on the ability to discern between *Batch* and *Shared* hypervisors we decided to restrict these experiments only to some representative methods form the two families: traditional and deep. The goal is to understand if the two user categories are significantly different from each other and at the same time measure the ability of the two families to capture patterns that go beyond the mean and variance.

In Figures 7.4, 7.5, 7.6 we report ROC and score distributions of the three scenarios tested on one window of data for four traditional methods (PCA, IForest, LOF, KNN) and two Deep Learning ones (Autoencoder Fully connected and CNN).

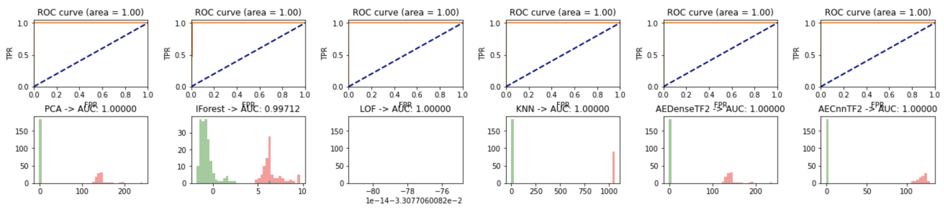


Figure 7.4: Unprocessed data. ROC and score distributions tested on one window of artificial setting with 183 *normal Batch hypervisors and* 91 *anomalous Shared hypervisors. Methods tested: PCA, IForest, LOF, KNN, Autoencoder Fully connected and CNN.*

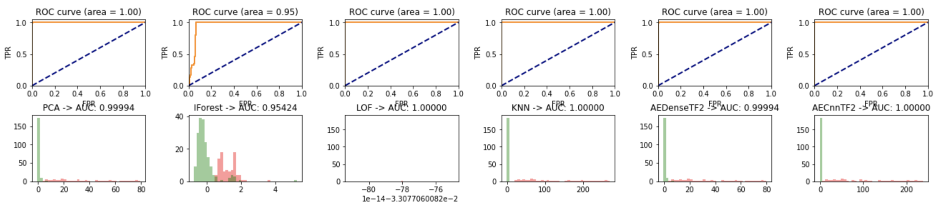


Figure 7.5: Same mean. ROC and score distribution tested on one window of artificial setting with 183 *normal Batch hypervisors and* 91 *anomalous Shared hypervisors. Methods tested: PCA, IForest, LOF, KNN, Autoencoder Fully connected and CNN.*

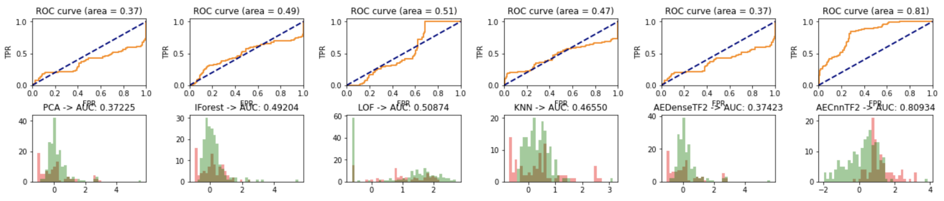


Figure 7.6: Same mean and Variance. ROC and score distribution tested on one window of artificial setting with 183 *normal Batch hypervisors and* 91 *anomalous Shared hypervisors. Methods tested: PCA, IForest, LOF, KNN, Autoencoder Fully connected and CNN.*

7.4 Algorithms' Implementation Details

For the majority of the Outlier Detection methods we relies on the implementation provided by PyOD [2] given the good level of code quality in terms of coverage and the support from the open source community. Note that for the three most popular traditional methods (LOF, iForest, OCSVM) the implementation of PyOD relies on the homonym classes from scikit-learn [3]. In the Table 7.3 every algorithm is paired with the library that implements it.

Algorithm Name	**Implementation**	**Version**
LOF	PyOD (scikit-learn)	0.8.0 (0.23.1)
IFOREST	PyOD (scikit-learn)	0.8.0 (0.23.1)
OCSVM	PyOD (scikit-learn)	0.8.0 (0.23.1)
PCA	PyOD	0.8.0
KNN	PyOD	0.8.0
ForecastVAR	this work	1.0
ForecastCNN	this work	1.0
AEFC	PyOD (adapted for TensorFlow 2 in this work)	0.8.0 (1.0)
AECC	this work	1.0
AELSTM	this work	1.0

Table 7.3: Algorithms used and their implementations

7.5 Final Results Discussion

We summarize in this section the main findings from the results of our three experiment: *Batch* dataset, *Shared* dataset and artificial setting. Firstly given the ease with which the anomaly detection methods can distinguish between the *Batch* and *Shared* hypervisors in the artificial setting (Figure 7.4), we can conclude that the two user categories are showing clearly different patterns in terms of both mean and variance (Figure 7.5). Therefore considering the two separate scenarios with two separate *Batch* and *Shared*

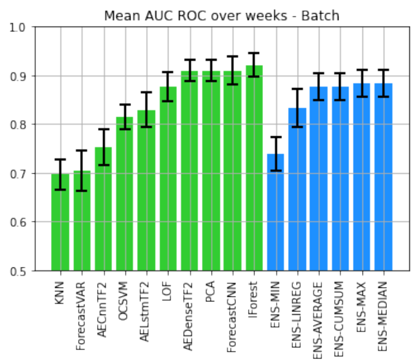
[2]Python Outlier Detection (PyOD) library, code available here: `https://github.com/yzhao062/pyod`

[3]scikit-learn library code available here: `https://github.com/scikit-learn/scikit-learn/`

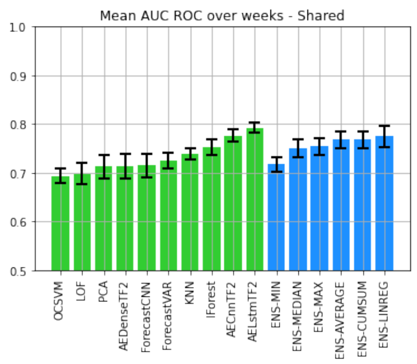
benchmark datasets is a reasonable choice and confirms the initial experts' belief.

7.5.1 Performance and Task Complexity

If we consider the mean AUC of the various methods in Figure 7.7 for the *Batch* and *Shared* datasets, we can clearly see that the *Batch* datasets lead to the higher AUC results. We can hereby confirm that the *Batch* scenario represents an easier task; moreover also the lack of significant difference between traditional and deep methods in this case can be seen as an indicator of an easier anomaly detection scenario in case of *Batch* hypervisor monitoring. We explain this difference also from visual inspection of the anomalies on the *Batch* that are usually corresponding to almost perfect step functions in the metrics, most of the time the CPU Load, whereas this is not the case for the *Shared* dataset.



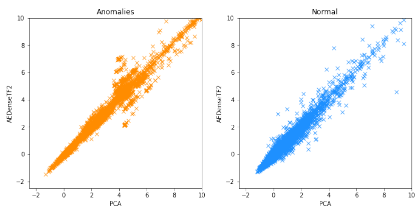
(a) *Batch* dataset



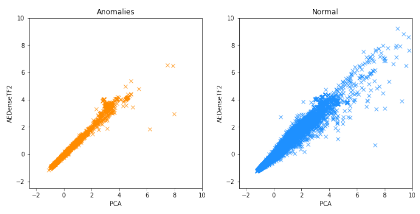
(b) *Shared* dataset

Figure 7.7: AUC-ROC all methods on Batch and Shared. It is computed as average over the weeks of analysis. The performance are sorted in increasing order and in green we can see the AUC of the traditional methods whereas in blue the ensemble strategies.

To reinforce this hypothesis that the *Batch* anomaly detection task probably does not need complex models to be solved we have that PCA performs incredibly well on par of other Deep learning methods like Autoencoder Fully Connected (AEDense). In fact, even if this deep model includes non linear activation functions it can still learn the linear solution of the problem. And the strong correlation between the PCA and AEDense anomaly scores in Figure 7.8 confirms the hypothesis that they converged on very similar solutions in both *Batch* and *Shared* dataset tasks. This good performance of the PCA is a good sign from a practical perspective, because it means that such a simple method can find most of the anomalies with a low False Positive Rate.



(a) *Batch* dataset



(b) *Shared* dataset

Figure 7.8: Anomaly scores correlation between Autoencoder Fully Connected and the PCA on both CERN curated dataset.

7.5.2 Input Data Quantity

The decision of subsampling the input for traditional methods prevents us from commenting on the training time difference between the traditional and deep families, but this choice is motivated by the fact that some of them are parametric and therefore do not learn any model but simply store the data showing in the end a poor scalability. On the performance side subsampling does not affect traditional methods as much as deep learning ones that if trained on smaller dataset lead to very miserable performance.

In terms of quantity of data required by the various methods we have two lesson learned in debugging problems with Autoencoder CNN and LOF methods respectively. We noticed that for the Autoencoder CNN in particular but also for other deep learning methods, learning on just non-overlapping windows of the previous week was not enough. In fact, that quantity of data for a common group of either *Batch* or *Shared* hypervisors contains around 4'200 windows and that is definitely not enough to cope with the need of Deep Learning methods. That is why we adopted the sliding windows approach in the training week. On the other hand for a traditional method like LOF, the usage of a disproportionately smaller number of neighbours than the size training set leads to a very poor result as shown in Figure 7.9

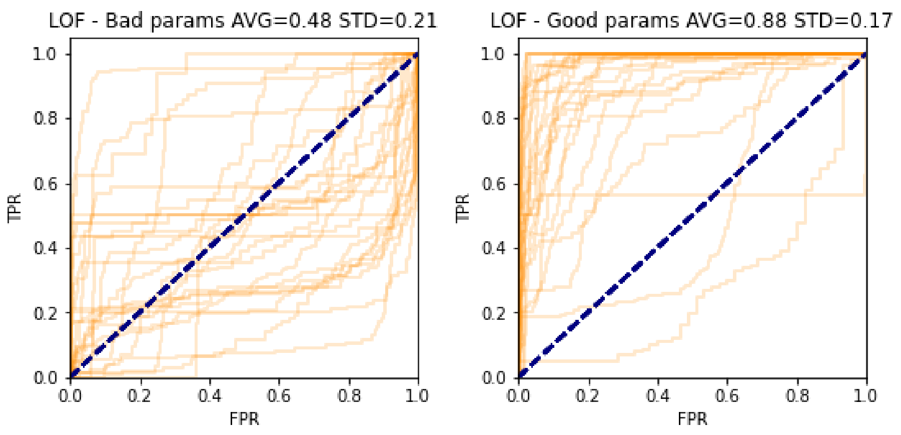


Figure 7.9: Example of bad and good LOF parametrization. In both cases we use as training set 1000 *samples. On the left we set the number of neighbours to* 20 *whereas on the right we set it to* 200

We therefore highlight the importance to appropriately set a number of neighbours based on the a validation dataset if possible.

7.5.3 Novel Methods Discussion

The new methods proposed based on the forecasting principle (ForecastVAR and ForecastCNN) show a different behaviour among themselves in terms of AUC performances on the *Batch* dataset, wherase they achieve similar ones in the more complex setting of *Shared* hypervisors. Even though the different model could be enough to justify this difference, we also argue that the subsampling step present in the ForecastVAR method could be partially responsible for this high variance in the *Batch* case. In fact the ForecastVAR methods subsample 20 of the overall ca 200 hypervisors of the group and makes a model on top of them, this phenomenon can be less visible in the *Shared* dataset since we only subsample for a group of 80 hypervisors.

On the other hand the ForecastCNN is the best among the Deep Learning group in the *Batch* and the second best in the *Shared* one. An important detail it is equivalent in term of AUC-ROC to the Autoencoder Fully Connected (AEDense) in both cases. This trend is confirmed in Figure 7.10 where we see a clear correlation between the two methods' anomaly scores, with the Autoencoder that tends to give a higher score to normal data whereas Forecast CNN gives consistently lower scores. The clear advantage of our model is in terms of model complexity: 632'048 parameters for the Autoencoder and only 2'803 for the Forecaster (Figure C.4 and C.1 of the Appendix). We can attribute this saving in parameters to the better suitability of Forecast CNN to handle temporal data. Nonetheless we also point out that Forecst CNN requires a sensibly longer training time (Figure 7.3).

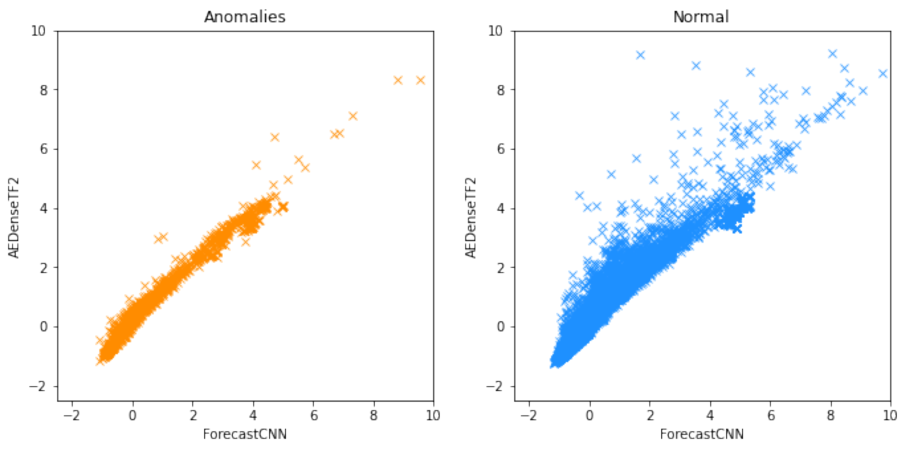


Figure 7.10: Anomaly scores correlation on the Shared dataset between Autoencoder Fully Connected and the Forecaster CNN.

Inspecting the results produced by the ensemble methods in Figure 7.7 we notice that most of the strategies are leading to similar AUC score with the exception of the min strategy that is clearly degrading the performance of the singular individuals. We can explain this with the fact that if at least one method in the ensemble is erroneously classifying a window as normal when it is not, this drives the entire ensemble to say that it is a normal sample. Therefore the min strategy is more sensitive to the worst method in the ensemble with a tendency to remove overlook anomalies. On the other hand the two methods analyzed and recommended by [45], namely max and average, are not showing particular different between each other in this context. On the contrary our novel ensemble method based on a simple Linear regression combination of the others and that is using a small amount of labels is able to achieve the highest score among the proposed ensemble strategies in the *Shared* scenario. We interpret it as a confirmation that also in a learner of second level the use of few labeled data can lead to superior performance in a similar way it happens usually thanks to outlier exposure in other Anomaly Detection methods [57].

Chapter 8

Conclusions

In this work we have tackled the problem of Anomaly Detection on Time Series data for the CERN large-scale computing infrastructure with both traditional Machine Learning algorithms and Deep Learning ones. The main contributions and outputs of this thesis are the following:

- **Dataset Collection**: we created two curated CERN datasets representing the problem of anomaly detection on time series on a large-scale computing infrastructure, with two levels of task complexity;
- **Comparative study**: we compared the performance of a selection of algorithms on the newly collected CERN datasets;
- **System Implementation**: we implemented a Proof of Concept Anomaly Detection system for the CERN Cloud Infrastructure.
- **Novel variants**: we propose two new variants Anomaly Detection methods on time series (Forecaster VAR and Forecaster CNN) together with a new combination strategy for an ensemble method.

From the experimental results we noticed how traditional methods are incredibly good at spotting anomalies in groups of hypervisors that are running similar batch jobs with the goal of fully utilize the computing resource. For this scenarios PCA, Local Outlier Factor and Isolation Forest methods are achieving the goal with a minimal training time. On the other side, when the hypervisors are used in an on-demand fashion by multiple users and services with intermittent jobs, then it is harder to achieve good performance on the anomaly detection task and Deep Learning methods have the power to have better performances than traditional methods if feed with enough data at training time. In particular architectures that model the temporal dimension, such as those LSTM-based, can outshine the traditional Fully Connected scenario.

Among the limitations of the current thesis work we highlight the following two points. The former is that we run our analysis following the expert opinion in most of our work, including the choice of metrics to monitor and the time frame of analysis. Nonetheless we believe that a systematic study on varying the number of input metrics and the time scale of analysis could have revealed respectively the robustness characteristic of the methods under study and the best time scale of analysis for the specific problem at hand. The second limitation is that we did not fully tuned every single method to perform at the best, but we use the default settings in most of the cases. A detailed parameter search could have revealed the best configuration for every method comparing them at the best of their possibility on the current task. We did not explored these two directions due to the lack of time and the need of having a prototype ready, even if in a Proof-of-Concept stage.

We therefore suggest some future directions that we would have explored with more time, in order of priority:

- explore the use of more metrics rather than the one suggested by the expert and with different time scales of analysis;
- explore alternative network architectures for the proposed Deep Learning models for maximizing their performance on the hardest setting of *Shared* group of hypervisors;
- thanks to the two new labelled CERN datasets, extend the comparative study including supervised techniques;
- thanks to the, now available, workflow to annotate time series in the monitoring infrastructure, explore active learning approaches to decide on which temporal windows are worth to be annotated first;
- use the data from multiple Openstack Groups to train more robust Deep Learning Models for the two user categories separately: one model for *Batch* and one for *Shared*; in these way we expect to learn from a larger pool of normal data and be more robust to small variation in the normal behaviour;
- explore a two steps procedure to combine the traditional machine Learning method and Deep Learning ones in a sequence to combine their strengths; for example, an Autoencoder architecture performs feature extraction and a traditional method detects anomalies in the new lower dimension feature space.

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Appendix A

Dataset

A.1 Overview Annotations

In this section we provide a visual overview of the annotations taken by the experts on the two datasets. We use a heatmap where every column represent an hypervisor whereas every row a window of data, note that we have 3 windows per day. We highlight with different colors the different types of windows:

- blue: normal window.
- orange: anomalous window.
- black: mixed (dropped for evaluation)
- white: no annotations provided by the expert on that window (dropped for evaluation).

For a precise description of every type of window refer to the Table 4.1 in the main text.

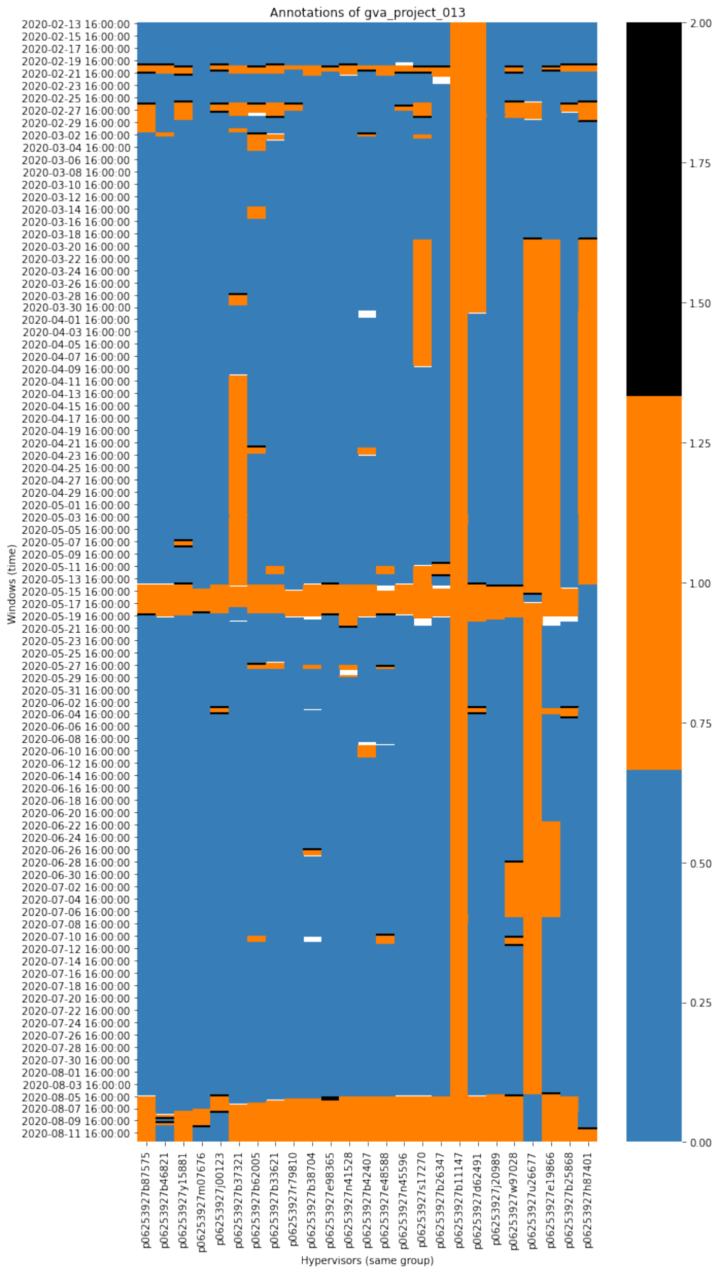


Figure A.1: Overview of Annotation Labels for Batch Openstack Cell: blue = normal, orange = anomaly, black = mixed, white = empty interval.

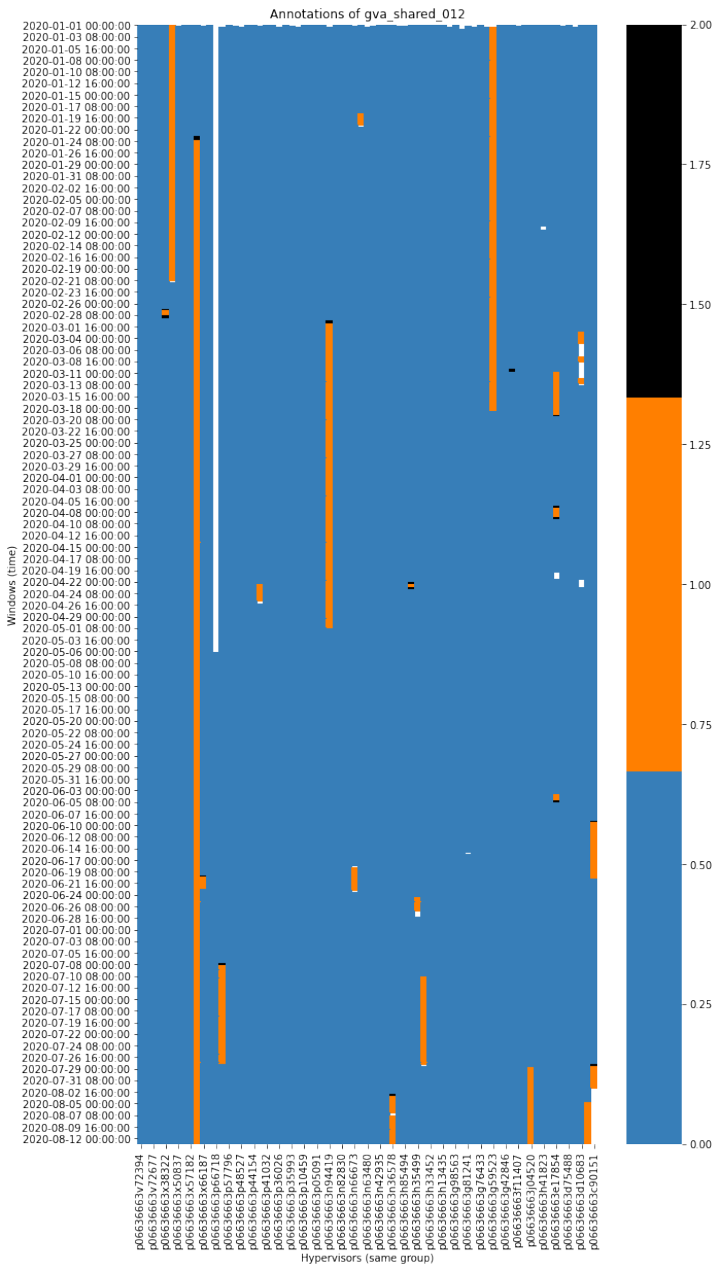


Figure A.2: Overview of Annotation Labels for Shared Openstack Cell: blue = normal, orange = anomaly, black = mixed, white = empty interval.

Appendix B

Complete Experiments' results

B.1 ROC and Performance Metrics: Complete Analysis

Next we show the results of the benchmark procedure of all the methods on the two curated datasets: for both *Batch* Dataset (Figures B.1 and B.2) and *Shared* Dataset (Figures B.3 and B.4).

B.2 Correlation of Anomaly Scores

In Figures B.5 and B.6 we show the comparison of the normalized anomaly scores of all algorithms with each other. Note that we analyse the correlation of scores of two algorithms in the range $[-2.5, 10]$ for both *Batch* and *Shared* dataset separately. Below the main diagonal we plot correlation among anomalous instances, whereas on the diagonal and above we visualise the normal samples.

B.3 Ensemble Performance

In Figures B.7 and B.8 we show the results of all the evaluated ensemble strategies: min, max, average, median, cumulative sum of all scores, linear regression combination (our method).

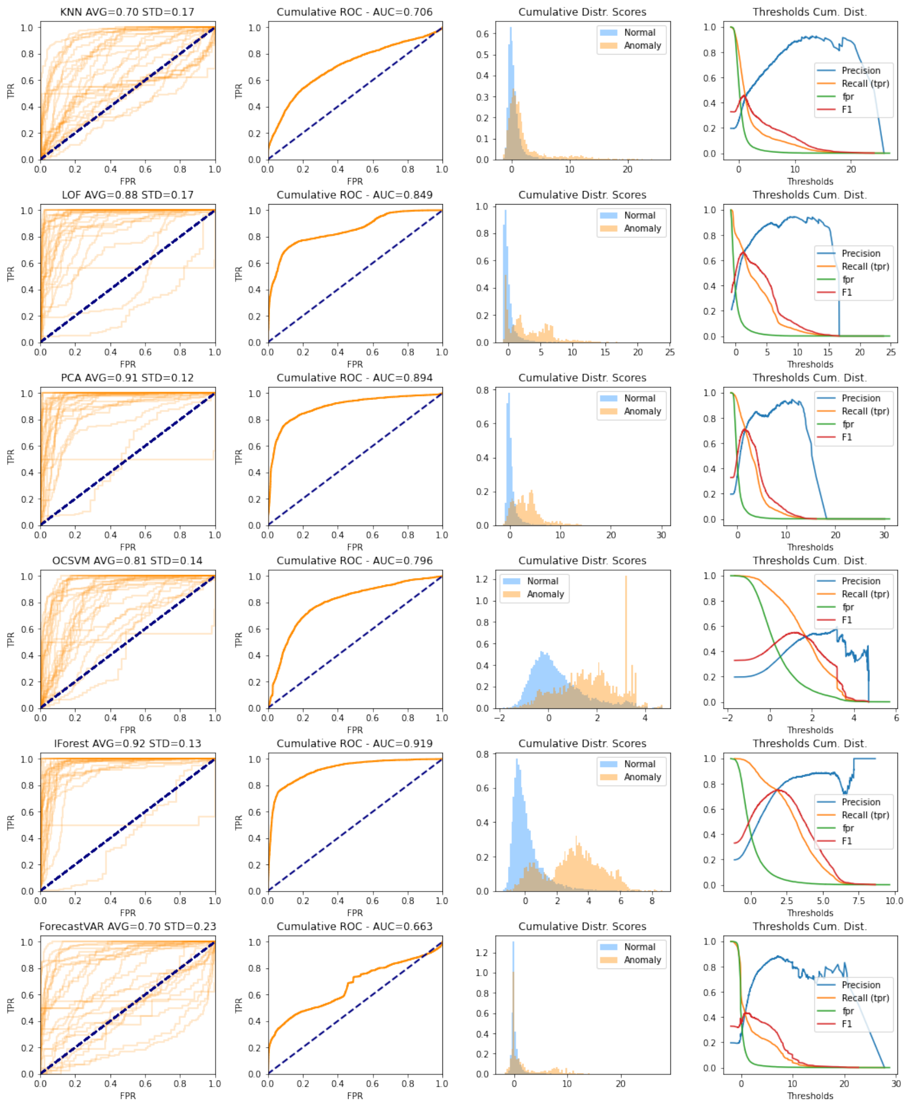


Figure B.1: Results on Batch dataset for Traditional Algorithms (KNN, LOF, PCA, OCSVM, IFOREST, ForecastVAR). The first column shows the multiple ROC curves build from the 26 weeks of data, the remaining represent cumulative quantities in which all weeks are represented together; we have in order the ROC, the cumulative distribution of anomaly scores and the performance metrics: Precision, Recall, False Positive Rate and F1.

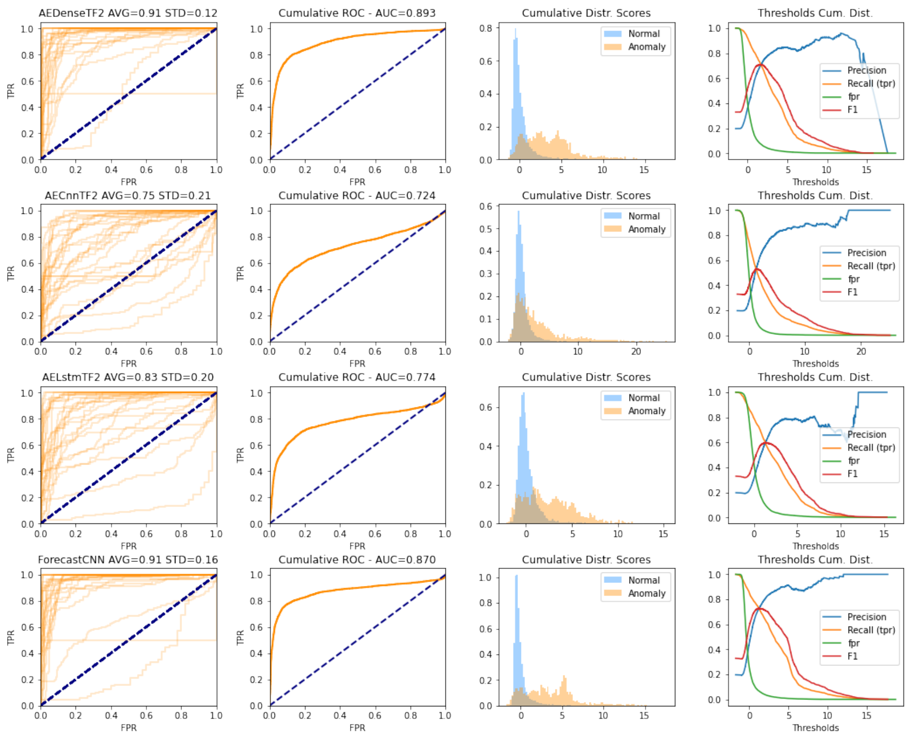


Figure B.2: Results on Batch dataset for Deep Algorithms (AEFC, AECNN, AELSTM, ForecastCNN). The first column shows the multiple ROC curves build from the 26 weeks of data, the remaining represent cumulative quantities in which all weeks are represented together; we have in order the ROC, the cumulative distribution of anomaly scores and the performance metrics: Precision, Recall, False Positive Rate and F1.

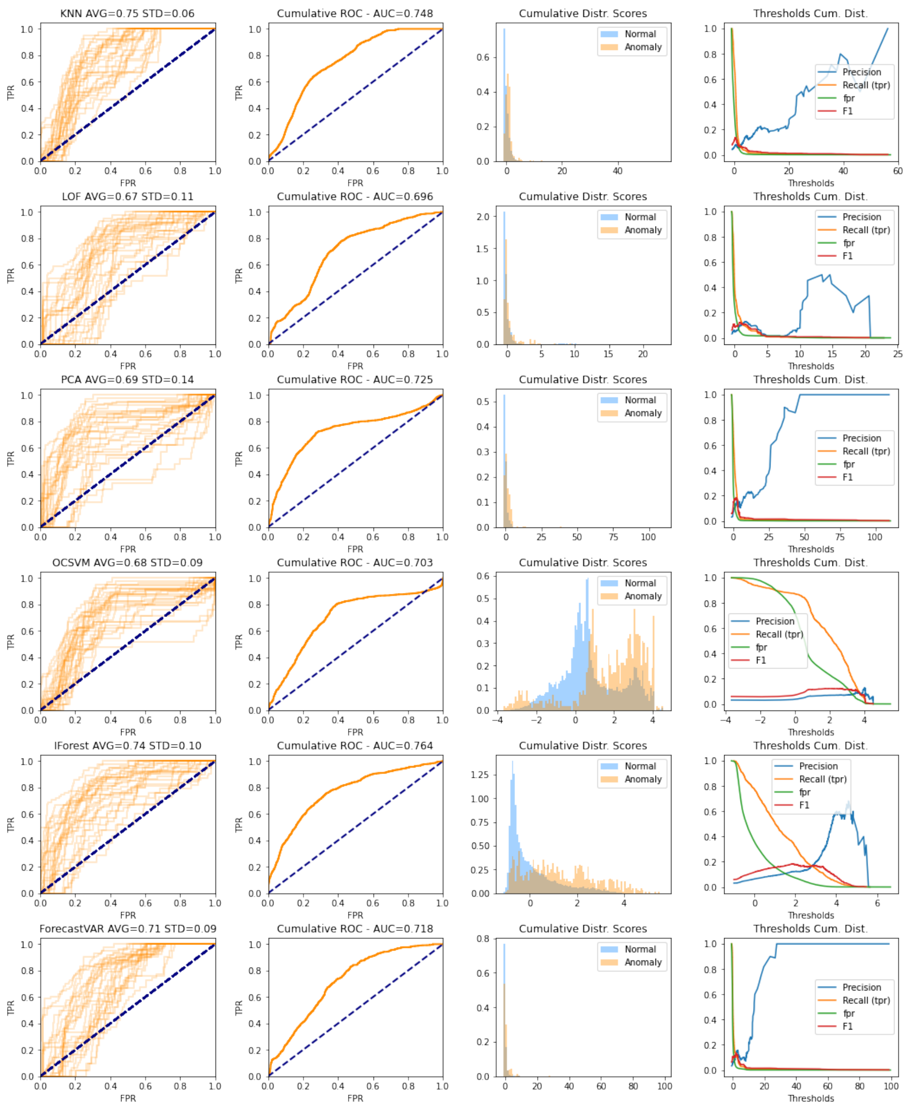


Figure B.3: Results on Shared dataset for Traditional Algorithms (KNN, LOF, PCA, OCSVM, IFOREST, ForecastVAR). The first column shows the multiple ROC curves build from the 32 weeks of data, the remaining represent cumulative quantities in which all weeks are represented together; we have in order the ROC, the cumulative distribution of anomaly scores and the performance metrics: Precision, Recall, False Positive Rate and F1.

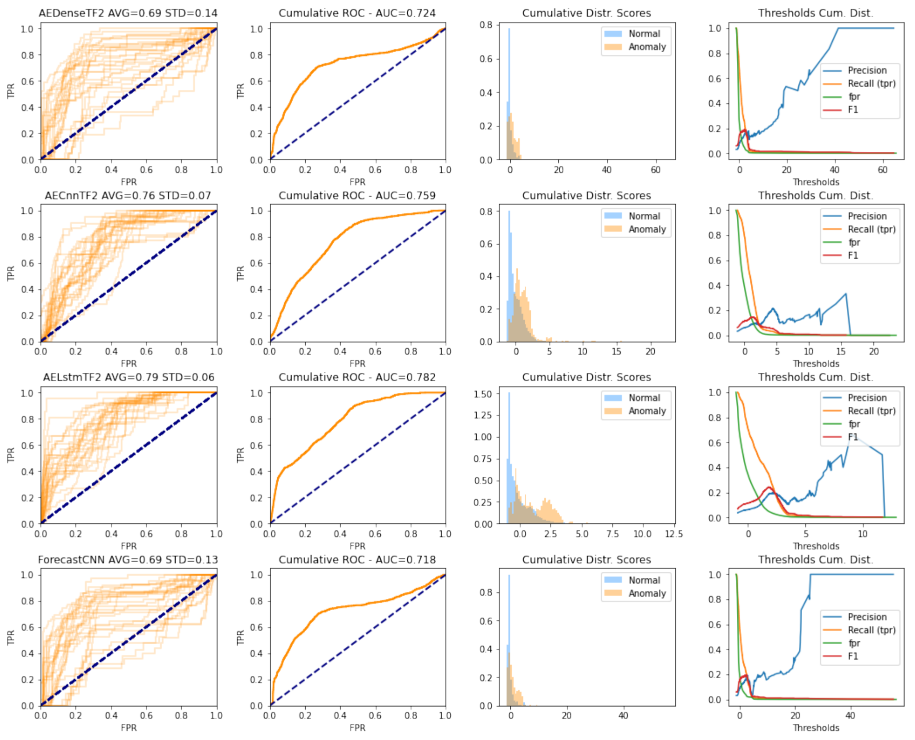


Figure B.4: Results on Shared dataset for Deep Algorithms (AEFC, AECNN, AELSTM, ForecastCNN). The first column shows the multiple ROC curves build from the 32 weeks of data, the remaining represent cumulative quantities in which all weeks are represented together; we have in order the ROC, the cumulative distribution of anomaly scores and the performance metrics: Precision, Recall, False Positive Rate and F1.

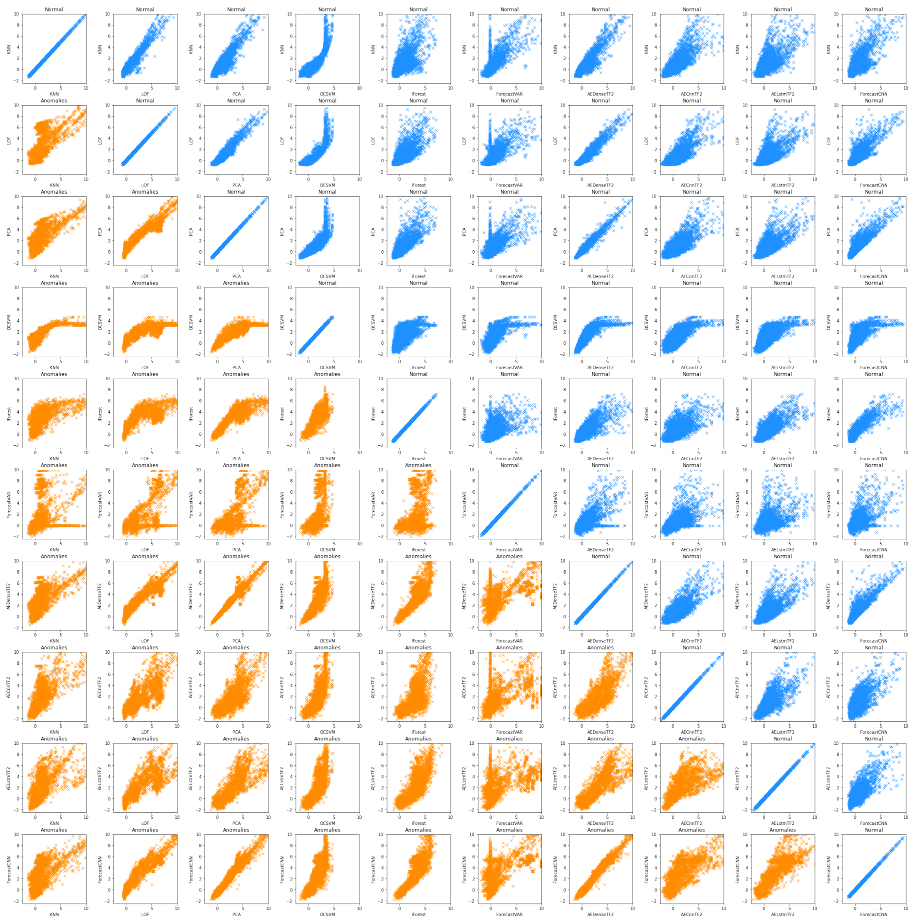


Figure B.5: Anomaly score correlation among all the pairs of algorithms for the Batch dataset. Below the main diagonal we have the anomalous instances, whereas on the diagonal and above we have the scores of normal instances.

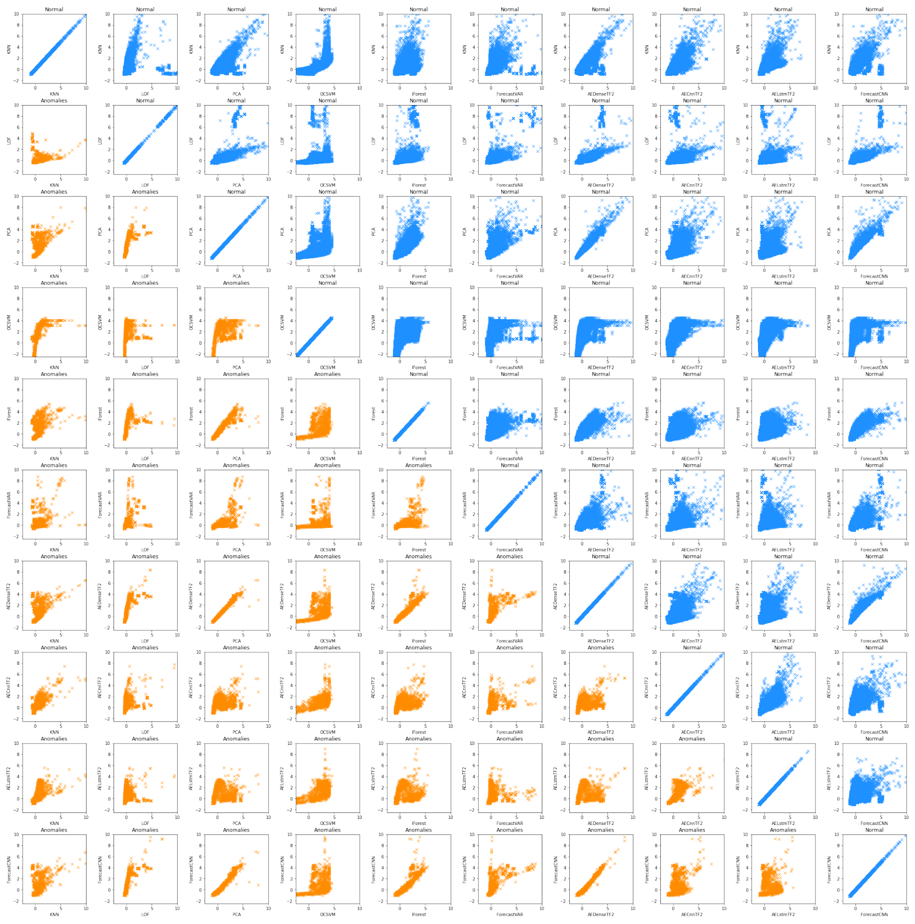


Figure B.6: Anomaly score correlation among all the pairs of algorithms for the Shared dataset. Below the main diagonal we have the anomalous instances, whereas on the diagonal and above we have the scores of normal instances.

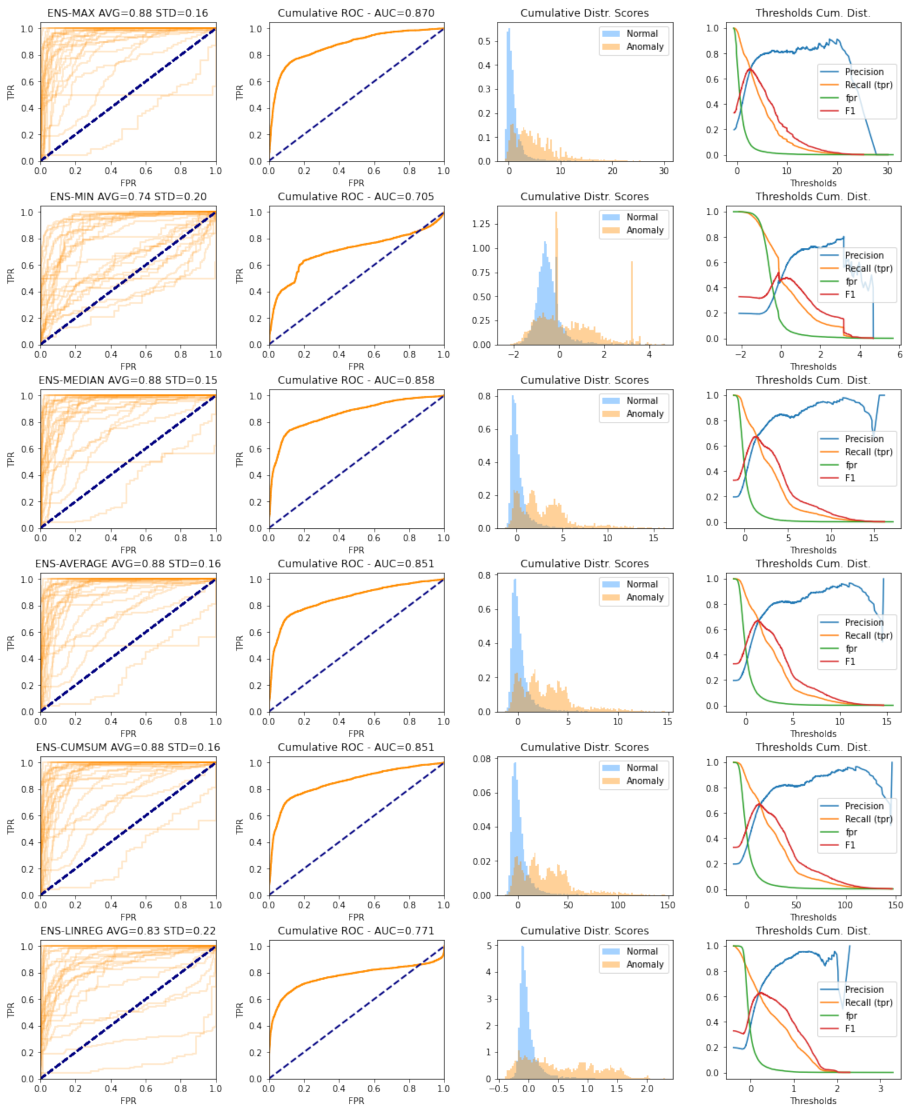


Figure B.7: Results on Batch dataset for Ensemble strategies (MIN, MAX, MED, AVG, CUMSUM, LINREG). The first column shows the multiple ROC curves build from the 26 weeks of data, the remaining represent cumulative quantities in which all weeks are represented together; we have in order the ROC, the cumulative distribution of anomaly scores and the performance metrics: Precision, Recall, False Positive Rate and F1.

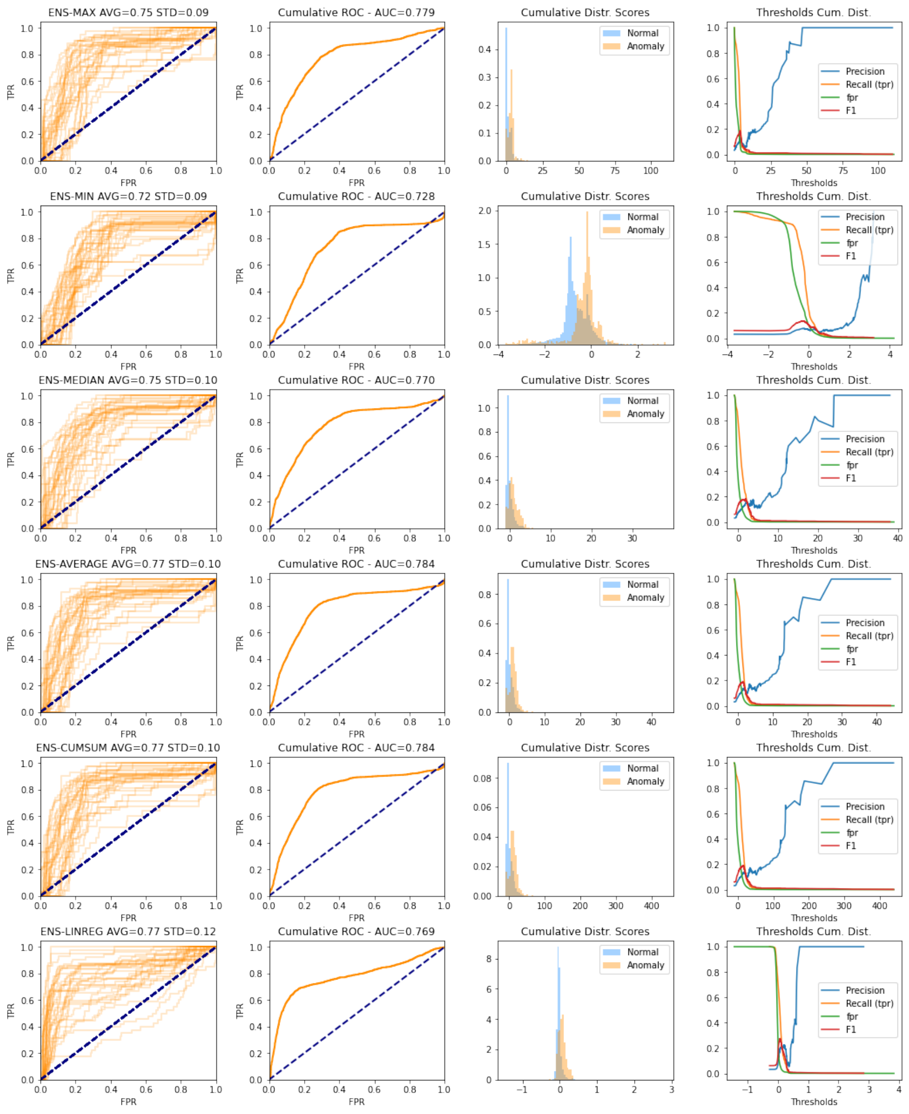


Figure B.8: Results on Shared dataset for Ensemble strategies (MIN, MAX, MED, AVG, CUMSUM, LINREG). The first column shows the multiple ROC curves build from the 32 weeks of data, the remaining represent cumulative quantities in which all weeks are represented together; we have in order the ROC, the cumulative distribution of anomaly scores and the performance metrics: Precision, Recall, False Positive Rate and F1.

Appendix C

Appendix

C.1 Code modification for Grafana Extension

Next we show the extension code for the client side Javascript of Grafana visualization platform.

```
// Get list of templated variables from the DOM
  var mylist = document.querySelectorAll('[aria-label="
    Dashboard template variables submenu item"]');
  //console.log(mylist);
  for (var i = 0; i < mylist.length; i++) {
   var mylabel = mylist[i].childNodes[0].childNodes[0].
    innerText;
   var myvalue = mylist[i].childNodes[0].childNodes[1].
    innerText;

   console.log("templated var label: " + mylabel);
   console.log("templated var value: " + myvalue);
   var mytag = mylabel + ":" + myvalue;
   console.log(mytag);
   //t.tags.push(myvalue);
   t.tags.push(mytag);
```

C.2 ElasticSearch Document Format

Next we show the json format of the document representing one candidate anomaly found by our algorithms and sent to the monitoring infrastructure to be stored in ElasticSearch and queried later in Grafana.

```
"algo": {
          "class_name": "PyODWrapperAnalyzer_IForest",
          "version": -1,
          "hparam_str": {},
      "hparam_int": {},
      "hparam_float": {},
      "hparam_bool": {}
    },
    "entity_data": {
      "entity": "p06253927b11147",
      "cell_name": "gva_project_013",
      "hostgroup": "cloud_compute/level2/batch/gva_project_013"
    },
    "entity_metrics": {
      "plugins": {
        "swap_swapfile_swap_used": {
          "type": "swap",
          "type_instance": "used",
          "plugin_name": "swap"
        },
        "swap_swapfile_swap_free": {
          "type": "swap",
          "type_instance": "free",
          "plugin_name": "swap"
        },
        "vmem__vmpage_io_memory_in": {
          "plugin_instance": "",
          "type": "vmpage_io",
          "type_instance": "memory",
          "value_instance": "in",
          "plugin_name": "vmem"
        },
        "vmem__vmpage_io_memory_out": {
          "plugin_instance": "",
          "type": "vmpage_io",
          "type_instance": "memory",
          "value_instance": "out",
          "plugin_name": "vmem"
        },
        "cpu__percent_user": {
          "plugin_instance": "",
          "type": "percent",
          "type_instance": "user",
          "plugin_name": "cpu"
        },
        "cpu__percent_idle": {
          "plugin_instance": "",
          "type": "percent",
          "type_instance": "idle",
          "plugin_name": "cpu"
        },
        "cpu__percent_system": {
          "plugin_instance": "",
          "type": "percent",
          "type_instance": "system",
          "plugin_name": "cpu"
        },
        "load_longterm": {
          "value_instance": "longterm",
          "plugin_name": "load"
        },
        "memory__memory_free": {
          "plugin_instance": "",
          "type": "memory",
          "type_instance": "free",
          "plugin_name": "memory"
        },
        "interface__if_octets__tx": {
          "type": "if_octets",
          "type_instance": "",
          "value_instance": "tx",
          "plugin_name": "interface"
        },
        "interface__if_octets__rx": {
          "type": "if_octets",
          "type_instance": "",
          "value_instance": "rx",
          "plugin_name": "interface"
        }
      }
    },
    "preprocessing": {
      "type": "standardization"
    },
    "temporal": {
      "time_start_milli": 1593583200000,
      "time_start": "2020-07-01T08:00:00.000Z",
      "time_end_milli": 1593612000000,
      "time_end": "2020-07-01T16:00:00.000Z",
      "window_length": 48,
      "step_resolution_minutes": 10
    },
    "anomaly": {
      "score": 3.9858576333577713,
      "rank_position": 1,
      "rank_percentile": 100,
      "explainalibilty": {
        "metric_0": "unsupported",
        "nr_anomalous_metrics": -1,
        "total_metrics": -1
      }
    },
    "is_anomaly": true,
    "slide_steps": 48,
    "ids": {
      "algo": "e5baa02f03953a43135216142ac60d0d38cf77e2",
      "entity_data": "f804e23d1862ac2eedcb4caacb179f223eb6a310",
      "entity_metrics": "970a503ce9349323e6651ce89ff84e1b6c302afb",
      "preprocessing": "61d6dbf3ad9cdca3b6a2e461ef5798d7b03a30bd",
      "temporal": "45d11d1f3987dd1998ee00264b0d5dd94ada2d28"
    },
    "document_id": "946169602798023d3d89db2380eaac11462b0521",
    "validity": true
```

C.3 Apache Spark - Big Data Preparation

This section contains the code used to prepare the data in the CERN Spark Cluster. We used the PySpark library to communicate with the cluster in Python code.

C.3.1 Data Reading

Next we show the code we use to read the data from HDFS and to keep only the hypervisors belonging to the Group of interest.

```python
def data_reading(spark, plugins, days, hostgroups):
    """Read all plugin and all days.

    Params
    ------
    spark: spark context
    plugins: dict.
        Every key is the signal name. Then inside it we have all the value for
        the colums necesary to filter the correct data.
    days: list of tuples
        every tuple is (year, month, day)
    hostgroups: list of str
        full paths for the hostrgoroups you are interested in

    Return
    ------
    all_data: PySpark DataFrame
```

```
        containing data from the plugins and cells in the following form:
        timestamp | hostname | hostgroup | value | plugin
        NB timestamp will be in seconds
        NB hostgroup is the the extended version
    """
    plugins = copy.deepcopy(plugins)
    inpaths = \
        create_paths_for_collectd(basepath="/project/monitoring/collectd",
                                  plugins=plugins, days=days)
    existing_inpaths = keep_only_existing_paths(spark=spark, paths=inpaths)
    [print(p) for p in sorted(existing_inpaths)]

    try:
        df_raw = spark.read.parquet(*existing_inpaths)
    except AnalysisException:
        print("path not found: %s" % existing_inpaths)
        return

    all_data =  \
        _keep_only_these_plugins_and_hg(df_raw, plugins, hostgroups)

    return all_data

def _keep_only_these_plugins_and_hg(df, plugins, hostgroups):
    """Keep only the plugins and hostgroups.

    Rename them also with the serialized version.
    """
    # filter hostgroups
    only_my_hgs = df.filter(F.col("submitter_hostgroup").isin(hostgroups))
    # create the filter string
    filter_str = ""
    # for every plugin create the condition and then put them in or
    # df.filter('d<5 and (col1 <> col3 or (col1 = col3 and col2 <> col4))')
    or_conditions = []
    # filter all the plugin individually
    for k in plugins.keys():
        plugin_dict = plugins[k]
        # for all attributes of this plugin
        and_conditions = []
        plugin_dict["plugin"] = plugin_dict.pop("plugin_name")
        for sub_k in plugin_dict.keys():
            value = plugin_dict[sub_k]
            and_conditions.append(sub_k + " == '" + value + "'"
    )
        plg_condition = "( " + " and ".join(and_conditions) + "
    )"
        # print("plg_condition: ", plg_condition)
        or_conditions.append(plg_condition)
    # print("or_conditions: ", or_conditions)

    # filter all interested line
    filter_str = " or ".join(or_conditions)
    print("filter_str: ", filter_str)
    only_my_plugins = only_my_hgs.filter(filter_str)

    df_list_plugin_ranamed = []
    # filter line of each plugin to rename them
    for plg_name, condition in zip(plugins.keys(),
    or_conditions):
        df_current = only_my_plugins.filter(condition)
        df_current = df_current.withColumn('plugin', F.lit(
    plg_name))
        df_list_plugin_ranamed.append(df_current)

    only_my_plugins_renamed = union_all(df_list_plugin_ranamed)

    # project only relevant column
    # cast timestamp to int (seconds)
    relevant_cols = only_my_plugins_renamed\
        .select("event_timestamp", "plugin",
                "host", "submitter_hostgroup", "value")\
        .withColumnRenamed("event_timestamp", "timestamp")\
        .withColumnRenamed("host", "hostname")\
        .withColumnRenamed("submitter_hostgroup", "hostgroup")\
        .withColumn("timestamp", (col("timestamp") / 1000).cast
    ("int"))

    return relevant_cols
```

C.3.2 Time Series/Metrics Aggregation

Next we show the code we use to summarize 10 minutes of consecutive data of a machine with the mean.

```
def downsampling_and_aggregate(spark, df_all_plugins,
    every_n_minutes):
    """Create the aggregate every x minutes.

    Example: if every 10 min it means that data between 15:10
    and 15:20 are
    summarized with the mean statistic and they will get
    timestamp 15:20.
    This happens for each hostname and plugin separately.

    Params
    ------
    spark: spark context
    df_all_plugins: PySpark DataFrame
        timestamp | hostname | hostgroup | value | plugin
    every_n_minutes: int
        nr of minutes you want to aggregate. The aggregation
    function is the
        average.

    Return
    ------
    aggregated_data: PySpark DataFrame
        containing data from the plugins and cells in the
    following form:
        timestamp | hostname | hostgroup | value | plugin
        NB timestamp will be in seconds
        Value contains the average values every x minutes for
    that host on that
        plugin.
    """
    aggregated_data = df_all_plugins\
        .withColumn(
            'minutes_group',
            F.col("timestamp") - (F.col("timestamp") % (60 *
    every_n_minutes))
        )\
        .withColumn('timestamp', F.col("minutes_group") + (60 *
     every_n_minutes))\
        .groupBy(['hostgroup', 'hostname', 'plugin', '
    minutes_group'])\
        .agg(
            F.mean('value').alias('value'),
            F.max("timestamp").alias("timestamp")
        )\
        .orderBy("timestamp")

    return aggregated_data
```

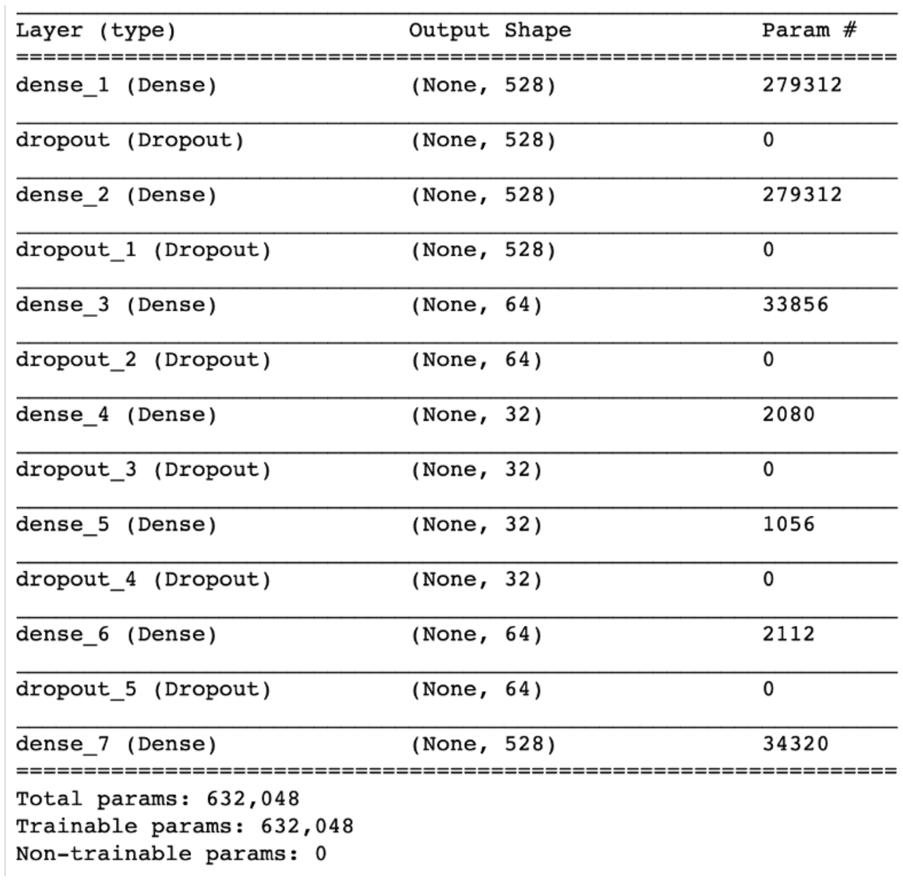
C.3.3 Time Series/Metric Normalization

Next we show the code we use to normalize the input data with respect to every single metric.

```
def normalize(spark, df, df_normalization):
    """Normalize the data given a dataframe with the coefficients.

    Remove the mean and divide by the std deviation to the value column.

    Params
    ------
    spark: spark context
    df: PySpark DataFrame
        timestamp | hostname | hostgroups | value | plugin
    df_normalization: PySpark DataFrame
        hostgroup | plugin | mean | stddev
        where mean and stddev are the mean and stddev of the relative plugin
        for the specified cell.

    Return
    ------
    normalized_data: PySpark DataFrame
        containing data from the plugins and cells in the following form:
        timestamp | hostname | hostgroup | value | plugin
        NB hostgroup is the the extended version
    """
    F.broadcast(df_normalization)
    to_be_normalized = df.join(df_normalization, ['hostgroup', 'plugin'])
    normalized_data = to_be_normalized\
        .withColumn("value",
                    (F.col("value") - F.col("mean")) / F.col("stddev"))\
        .select("timestamp", "hostname", "hostgroup", "plugin", "value")

    return normalized_data
```

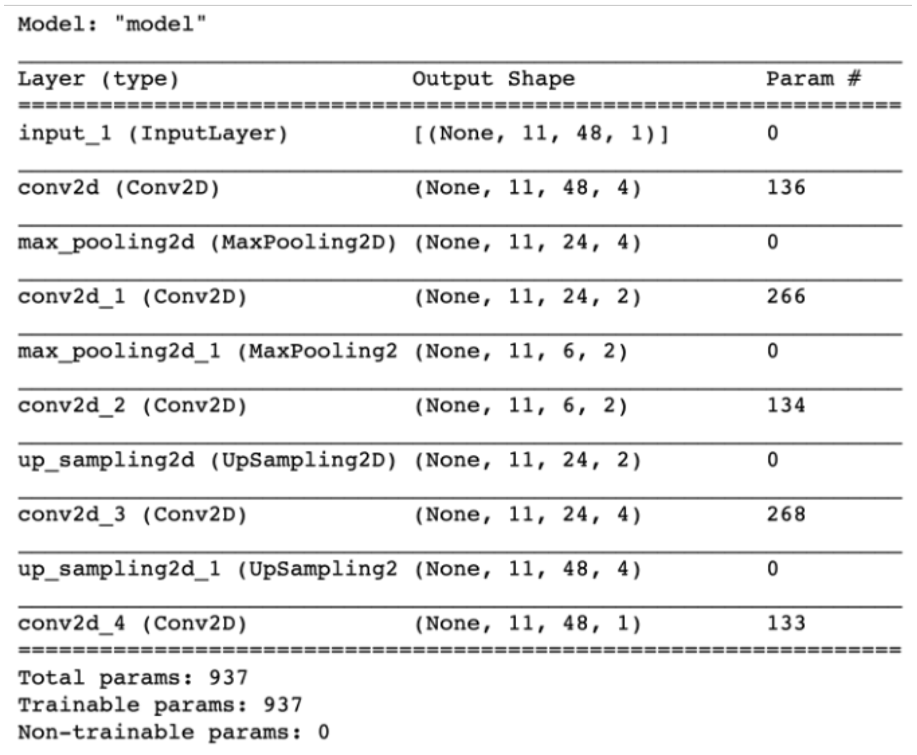
C.4 Deep Learning Architecture details

In this section we summarize the details of all the four deep methods with the TensorFlow summary tool that gives us information about the structure and type of layer. An important information is also the number of parameters of the overall model that gives us an idea of its complexity.



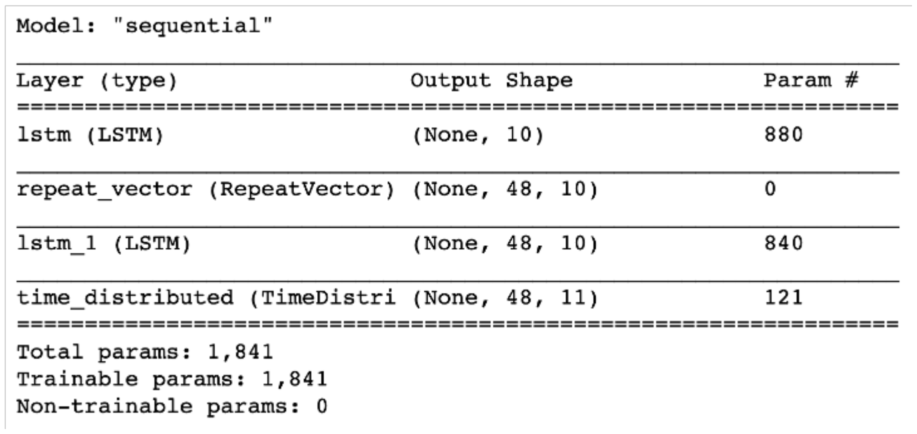
```
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_1 (Dense)              (None, 528)               279312
_________________________________________________________________
dropout (Dropout)            (None, 528)               0
_________________________________________________________________
dense_2 (Dense)              (None, 528)               279312
_________________________________________________________________
dropout_1 (Dropout)          (None, 528)               0
_________________________________________________________________
dense_3 (Dense)              (None, 64)                33856
_________________________________________________________________
dropout_2 (Dropout)          (None, 64)                0
_________________________________________________________________
dense_4 (Dense)              (None, 32)                2080
_________________________________________________________________
dropout_3 (Dropout)          (None, 32)                0
_________________________________________________________________
dense_5 (Dense)              (None, 32)                1056
_________________________________________________________________
dropout_4 (Dropout)          (None, 32)                0
_________________________________________________________________
dense_6 (Dense)              (None, 64)                2112
_________________________________________________________________
dropout_5 (Dropout)          (None, 64)                0
_________________________________________________________________
dense_7 (Dense)              (None, 528)               34320
=================================================================
Total params: 632,048
Trainable params: 632,048
Non-trainable params: 0
```

Figure C.1: Tensorflow Summary of the Autoencoder Fully Connected



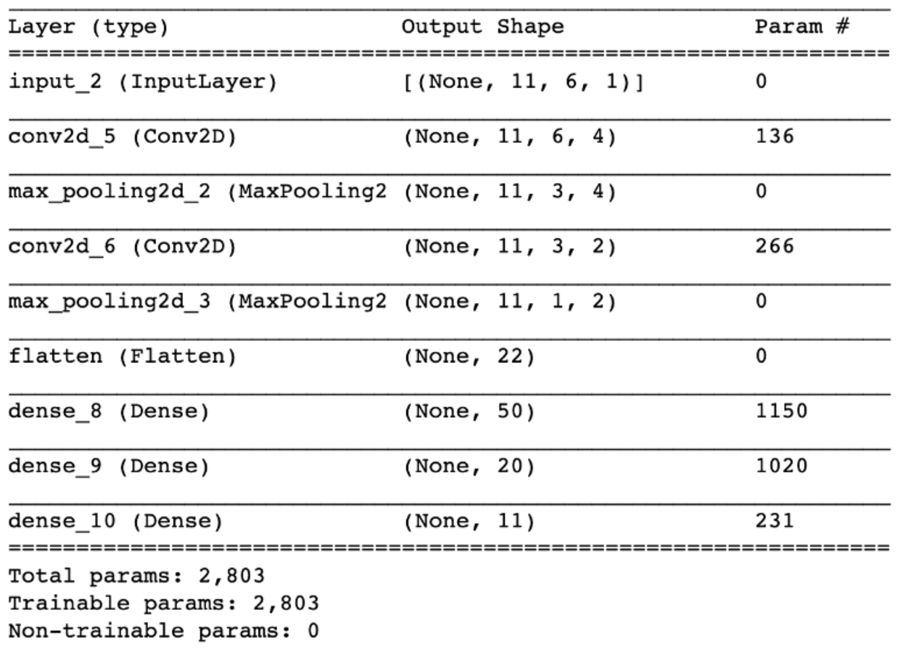
```
Model: "model"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
input_1 (InputLayer)         [(None, 11, 48, 1)]       0
_________________________________________________________________
conv2d (Conv2D)              (None, 11, 48, 4)         136
_________________________________________________________________
max_pooling2d (MaxPooling2D) (None, 11, 24, 4)         0
_________________________________________________________________
conv2d_1 (Conv2D)            (None, 11, 24, 2)         266
_________________________________________________________________
max_pooling2d_1 (MaxPooling2 (None, 11, 6, 2)          0
_________________________________________________________________
conv2d_2 (Conv2D)            (None, 11, 6, 2)          134
_________________________________________________________________
up_sampling2d (UpSampling2D) (None, 11, 24, 2)         0
_________________________________________________________________
conv2d_3 (Conv2D)            (None, 11, 24, 4)         268
_________________________________________________________________
up_sampling2d_1 (UpSampling2 (None, 11, 48, 4)         0
_________________________________________________________________
conv2d_4 (Conv2D)            (None, 11, 48, 1)         133
=================================================================
Total params: 937
Trainable params: 937
Non-trainable params: 0
```

Figure C.2: Tensorflow Summary of the Autoencoder CNN



```
Model: "sequential"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
lstm (LSTM)                  (None, 10)                880
_________________________________________________________________
repeat_vector (RepeatVector) (None, 48, 10)            0
_________________________________________________________________
lstm_1 (LSTM)                (None, 48, 10)            840
_________________________________________________________________
time_distributed (TimeDistri (None, 48, 11)            121
=================================================================
Total params: 1,841
Trainable params: 1,841
Non-trainable params: 0
```

Figure C.3: Tensorflow Summary of the Autoencoder LSTM



```
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
input_2 (InputLayer)         [(None, 11, 6, 1)]        0
_________________________________________________________________
conv2d_5 (Conv2D)            (None, 11, 6, 4)          136
_________________________________________________________________
max_pooling2d_2 (MaxPooling2 (None, 11, 3, 4)          0
_________________________________________________________________
conv2d_6 (Conv2D)            (None, 11, 3, 2)          266
_________________________________________________________________
max_pooling2d_3 (MaxPooling2 (None, 11, 1, 2)          0
_________________________________________________________________
flatten (Flatten)            (None, 22)                0
_________________________________________________________________
dense_8 (Dense)              (None, 50)                1150
_________________________________________________________________
dense_9 (Dense)              (None, 20)                1020
_________________________________________________________________
dense_10 (Dense)             (None, 11)                231
=================================================================
Total params: 2,803
Trainable params: 2,803
Non-trainable params: 0
```

Figure C.4: Tensorflow Summary of the Forecast CNN

C.5 Image Credits

The icon representing a normal and faulty robots come from freepik from Flaticon.com

- www.flaticon.com/-iconrobot_3398611
- www.flaticon.comfree-iconrobot_3398643