

FACHHOCHSCHULE NORDWESTSCHWEIZ

MASTER THESIS PROPOSAL

Thesis Title

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in the*

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Declaration of Authorship

I, Kevin SANER, declare that this thesis titled, “Thesis Title” and the work presented in it are my own. I confirm that:

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- Where I have consulted the published work of others, this is always clearly attributed.
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“Your brain does not manufacture thoughts. Your thoughts shape neural networks.”

Deepak Chopra

FACHHOCHSCHULE NORDWESTSCHWEIZ

Abstract

School of Business

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Thesis Title

by Kevin SANER

The Thesis Abstract is written here (and usually kept to just this page). The page is kept centered vertically so can expand into the blank space above the title too...

Acknowledgements

The acknowledgments and the people to thank go here.

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List of Abbreviations

DNN	D eep N eural N etwork
CNN	C onvolutional N eural N etwork
RNN	R ecurrent N eural N etwork
GRU	G ated R ecurrent U nit N etwork
LSTM	L ong S hort T erm M emory
AUC	A rea U nder the C urve

For/Dedicated to/To my...

Chapter 1

Introduction

With the rise of the Internet of Things (IoT) and ever more sensors, gadgets and smart devices like smartwatches for fall detection or blood pressure monitoring, or fridges for temperature protective control in use, the amount of available data steadily increases (Alansari et al., 2018). Simultaneously, the possibilities to use the data to draw conclusions increases. This data is generally used to draw conclusions such as failure of a system or a medical issue, such as a heart attack. These events typically occur very rarely (Hauskrecht et al., 2007). However, when the number of instances of each class is approximately equal, most machine learning algorithms function best. Problems occur when the number of instances of one class greatly exceeds the number of instances of the other. This issue is very popular in practice, and it can be observed in a variety of fields such as fraud detection, medical diagnosis, oil spillage detection, facial recognition, and so on (Thabtah et al., 2020). The task of identifying the rare item, event or observation is often referred to as anomaly detection. Typically, the anomalous item translates to problems such as bank fraud or medical problems. Often, the anomaly does not adhere to the common statistical definition of an outlier. Therefore, many outlier detection methods (in particular unsupervised methods) fail on such data (Hodge and Austin, 2004).

A special discipline in anomaly detection is to find the anomaly in a time series. The anomaly detection problem for time series is usually formulated as finding outlier data points relative to some standard or usual signal. Time series anomaly detection plays a critical role in automated monitoring systems. It is an increasingly important topic today, because of its wider application in the context of the Internet of Things (IoT), especially in industrial environments. The most popular techniques to find the anomalies are:

- Statistical Methods
- Support Vector Machines
- Clustering
- Density-based Techniques
- Neural Networks

Currently Neural Networks are regarded the cutting-edge research. Although first approaches to use artificial neural networks exist since 1969. They are popular in research for only about 15 to 20 years, which is why scientist generally expect further improvements on this kind of technology. This promising outlook is why this research paper also purely focusses on Neural Networks for anomaly detection. Especially Recurrent Neural Networks and Convolutional Neural Networks are investigated and compared.

1.1 Definitions

Following, the most important terms in the context of anomaly detection using neural networks are elaborated and defined.

1.1.1 Univariate, Bivariate and Multivariate Data

Time series data investigation poses a special discipline. Generally anomalies in time series are harder to detect for traditional statistical models, since the possibility of long term dependencies exist. Time series data comes in different forms. It is distinguished between univariate, bivariate and multivariate data. Univariate involves the analysis of a single variable while bivariate and multivariate analysis examines two or more variables. One significant difference between time-series and other datasets is that the observations are dependent not only on the components d , but also on the time feature n . Thus, time-series analysis and the statistical methods employed are largely distinct from methods employed for random variables, which assume independence and constant variance of the random variables. Time-series are important to data analysts in a variety of fields such as the economy, healthcare and medical research, trading, engineering, and geophysics. These data are used for forecasting and detecting anomalies.

Univariate Data

There is only one variable in this type of data. Because the information only deals with one variable that changes, univariate data analysis is the simplest type of analysis. It is not concerned with causes or relationships, and the primary goal of the analysis is to describe the data and identify patterns.

Bivariate Data

This type of data involves two different variables. This type of data analysis is concerned with causes and relationships, and the goal is to determine the relationship between the two variables.

Multivariate Data

Multivariate data is defined as data that contains three or more variables. It's similar to bivariate, but there are more dependent variables meaning there is not only one variable that influences the observed behavior (independent variable) but several. The methods for analyzing this data are determined by the objectives to be met. Regression analysis, path analysis, factor analysis, and multivariate analysis of variance are some of the techniques. Data collected from several sensors installed in a car is an example of a multivariate time-series.

1.1.2 Neural Networks

An Artificial Neural Network (ANN) with several layers between the input and output layers, is known as a Deep Neural Network (DNN). Neural networks come in a variety of shapes and sizes, but they all have the same basic components: neurons, weights and functions. These components work in a similar way as human brains and can be trained just like any other machine learning algorithm.

Neuron

Artificial neurons represent the smallest building blocks of neural networks. A neuron usually receives separately weighted inputs which it sums. The sum is then passed through the activation function to calculate the output of the neuron. When training a neural network, the input weights are adjusted by the optimizer function to improve accuracy of the given task e.g. classification.

Layer

In neural networks three different kind of layers are distinguished. There are input, output and hidden layers. A layer can be described as a collection of neurons. All layers between the input and output layer are called hidden layers. In the input layer data is fed into the neural network. The output of the hidden layer is calculated by taking the weighted sums of input and passing it through the activation function. Typically, a more complex problem requires more hidden layers to accurately calculate the output. In the output layer the final result e.g. a classification is produced. Figure 1.1 how a simple Neural Network with just one hidden layer could look like.

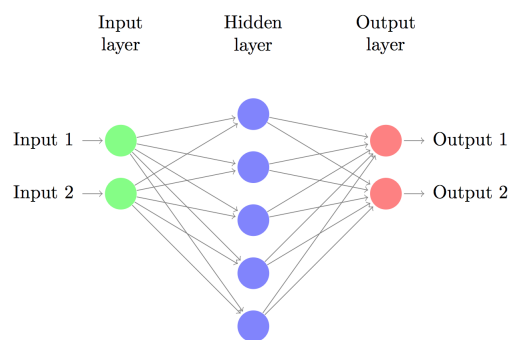


FIGURE 1.1: Input, Hidden and Output Layers (Denny Britz, 2015)

Optimizer Function

1.2 Background

Following, it is explained how different kinds of neural networks work and what they are used for.

1.2.1 Neural Networks for Anomaly Detection

Out of the three most popular neural network architectures, convolutional neural networks (CNN), recurrent neural networks (RNN) and deep neural networks (DNN), only RNN are typically used for anomaly detection in time series. RNNs have built-in memory and are therefore able to anticipate the next value in a time series based on current and past data. Classic or vanilla RNNs can theoretically keep track of arbitrary long-term dependencies in input sequences. There, however, is a computational issue: when using back-propagation to train a vanilla RNN, the back-propagated gradients can "vanish" or "explode" due to the computations involved in

the process, which use finite-precision numbers. Because LSTM units allow gradients to flow unchanged, RNNs using LSTM unit or Gated Recurrent units (GRU) partially solve the vanishing gradient problem and therefore drastically improve accuracy (Hochreiter and Schmidhuber, 1997).

Specially to mention in this context are LSTM (Long-Short Term Memory) and GRU (Gated Recurrent Units). Both achieved outstanding performance when used for tasks such as unsegmented, connected handwriting recognition, speech recognition and anomaly detection in network traffic or IDSs (intrusion detection systems) (Chung et al., 2014)

LSTM

LSTM was first proposed in 1997 by Schmidhuber and Hochreiter (Hochreiter and Schmidhuber, 1997). The initial version to the LSTM unit consisted of a cells, input and output gates. In 1999, the LSTM architecture was improved by introducing a forget gate and therefore allowing the LSTM to reset its own state (Gers, Schmidhuber, and Cummins, 2000). LSTM is used in a supervised training approach, that means it tries to predict a predefined state taking the past and the current state. If the predicted state differs from the expected state, the weights of the different gates are adjusted using an optimizer algorithm such as gradient descent. Figure 1.2 shows how the gates and the cell are arranged. The cell represents the memory of the LSTM. In simple words, the LSTM works as follows to predict a new value:

1. Forget Gate: Obsolete information is removed from the cell state.
2. Input Gate: New information is added to the cell state
3. Output Gate: The new information and the cell state are added to make the new prediction.
4. The new cell state is propagated to the next LSTM unit

CNN

In contrast to RNNs Convolutional Neural Networks are generally used for image classification. CNNs work as feature extractors and are able to recognize patterns . CNNs use layers that are not fully connected, to reduce complexity (compare to 1.2.1). In a CNN, a set number of neurons forms a filter. These filters or kernels are the actual feature extractors. A filter may represent a line or pattern (see Figure 1.3) (LeCun et al., 1998).

To detect whether, a feature is occurrent in a picture, the filter is gradually moved over the picture in so called strides. In every step (stride) the dot-product between the filter and the part of the picture is calculated. The results of the operations are stored in activation maps. The greater the dot-product the more alike are the filter and the section of the image. Training the network hereby refers to determining the shapes of these filters. Other typical features of a CNN are the pooling layers. The pooling layers reduce the amount of computation necessary. The most commonly used pooling technique is max-pooling and works as shown in Figure 1.4.

The idea of max-pooling is to only keep the maximum value of an activation map. In the orange region 7 represents the maximum value, so it is kept while the other values are discarded (Rich Stureborg, 2019).

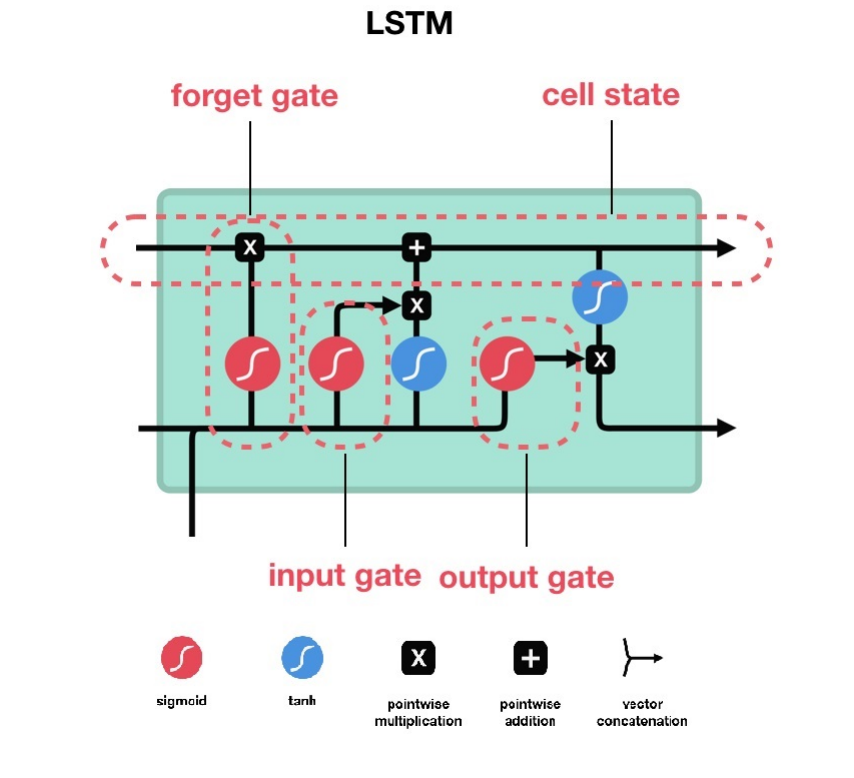


FIGURE 1.2: Gates and Cell of LSTM (Michael Phi, 2018)

In 2019, Wen and Keys proposed to use CNN also for anomaly detection in time series since it shares many common aspects with image segmentation. A univariate time series is therefore viewed as a one-dimensional image.

1.2.2 Transfer Learning

The reuse of a previously trained model on a new problem is known as transfer learning. It is currently very popular in deep learning because it can train deep neural networks with a relatively small amount of data. This is particularly useful in the field of data science, as most real-world problems do not provide millions of labeled data points to train complex models. In transfer learning, the knowledge of an already trained machine learning model is applied to a different but related problem. For example, if a classifier was trained to predict if an image contains a backpack, the model's experience could be applied to recognize other objects such as sunglasses (Niklas Donges, 2020).

1.3 Problem Statement

Defining a ground truth is one of the most difficult aspects of time series anomaly detection. Determining when anomalous behavior begins and ends in time series is a difficult task, as even human experts are likely to disagree in their assessments. Furthermore, there is the question of what constitutes a useful detection when detecting anomalies in time series. In the past, RNN have successfully been used for

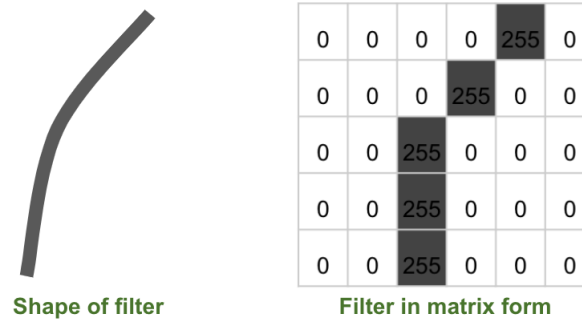


FIGURE 1.3: Example of a Filter used in CNN

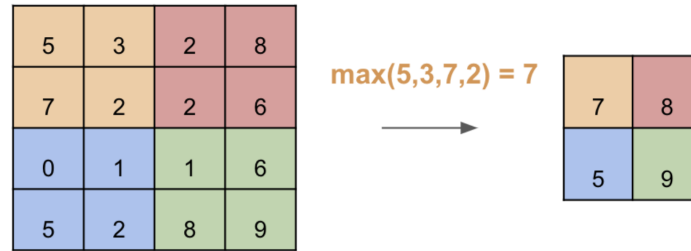


FIGURE 1.4: Example of max-pooling

anomaly detection (e.g. [(Malhotra et al., 2015); (Fan et al., 2016)]). Therefore, designs for various use cases are well researched. RNN are well suited for the task, however, take a long time to train due to the complexity of how a single unit is designed (see 1.2.1). In comparison CNN are not as complex and therefore, generally take less time to train. However, CNNs are generally used for image recognition and were only very recently used for anomaly detection in time series. It is therefore mostly unknown what designs are applicable for successful anomaly detection in time series data. While RNN are able to deal with multivariate data by design, a classical CNN requires design changes to be able to deal with multivariate data. Wen and Keys (2019) proposed to use a special kind of U-net, an improved version of a Fully Convolutional Neural Network (Ronneberger, Fischer, and Brox, 2015). Further, a CNN is not capable to analyze streaming data so it relies on segmentation of the data. These data segments are called snapshots. In order to not miss any data points, the frequency of taking these snapshots should be at least as high as the length of snapshot so that every time point is evaluated by the model at least once. However, for better performance it might prove beneficial to use a higher frequency which means every point is evaluated various times by the model (Wen and Keyes, 2019). The proposed design change and the fact that every point is evaluated multiple times, increases complexity and evaluation time and therefore counteract the architectural advantage of CNN compared to a RNN. When designing a neural network many parameters have to be chosen, this applies to both mentioned types of Neural Networks. For example, when designing a CNN, the number of layers, the activation function(s) of a single neuron and the optimizer function have to be chosen. Additionally, when using CNN for time series data the length and frequency of the snapshots have to be determined. Similarly, when designing a RNN also the number of layers and the optimizer function have to be determined. Because the basic building blocks of both networks types are very different it is difficult to fairly

compare the complexity of two architecture approaches. Another important parameter which applies to both network types is the number of epochs for which the networks are trained. Through the epochs the training time is determined. In order to compare the two types of neural networks, two networks of similar complexity have to be designed. With equal training time the performance of both can be compared and evaluated. A RNN is therefore only set up as benchmark while the main goal of this research project is to clarify whether CNNs are really useful and propose an advantage over RNNs when applied on time series data for anomaly detection.

1.4 Thesis Statement

Convolutional Neural Networks are superior to Recurrent Neural Networks when looking for anomalies in time series data regarding training time and complexity.

1.4.1 Subquestions

- How does a CNN for univariate and multivariate data need to be designed for successful anomaly detection in time series data?
- What advantages and disadvantages arise when using a CNN compared to a RNN for anomaly detection in univariate and multivariate time series?
- What parameter settings are crucial for a fair performance comparison between RNN and CNN?
- Optional: How does transfer learning affect the performance of CNN compared to RNN in anomaly detection in time series?

1.4.2 Research Objectives

Following the research objectives of this paper are defined.

1. Determine what design changes a CNN requires to detect anomalies in time series data.
2. Determine how the CNN should be designed for the comparison with a RNN
3. State the advantages and disadvantages of the chosen CNN architecture.
4. Define parameters which allow a fair comparison of CNN and RNN

1.4.3 Limitations

Recently there have been approaches that combine CNN and RNN into a hybrid network for tasks such as handwriting recognition or video-based emotion recognition (Dutta et al., 2018) (Fan et al., 2016). However, this paper only compares pure CNN and RNN, and does investigate a hybrid approach.

1.4.4 Significance

Until now, time series data was almost only approached with RNNs. This paper should answer the question whether CNNs propose a valid alternative and even propose some advantages over RNNs. The paper will answer the fundamental question whether research should channel efforts to further investigate CNNs for anomaly detection in time series data or whether no benefits can be discovered and research is better to focus on other areas.

1.4.5 Chapter Overview

Chapter 2

Related Literature

2.1 Anomaly or Outlier?

Generally, there is no agreement on how to distinguish between anomalies and outliers. The following often used citation proves equality of the term outliers and anomalies.

“Outliers are also referred to as abnormalities, discordants, deviants, or anomalies in the data mining and statistics literature.” - Aggarwal (2013)

By others, outliers are regarded as corruption in data, while anomalies are abnormal points with a particular pattern. In the context of this paper, only the term anomaly is used to refer to such irregular behaviour. It is hereby important to provide a clear definition for the concept of anomaly. This is critical since different meanings of abnormalities necessitate different detection methods. As a result, it is important to identify the key characteristics of anomalies and to use the description to highlight the boundaries. Following, two of the most common definitions of anomalies:

“Anomalies are patterns in data that do not conform to a well defined notion of normal behavior.” - Chandola et al. (2009)

Ord (1996), defines anomalies as follows:

“An observation (or subset of observations) which appears to be inconsistent with the remainder of that set of data.”

Anomalies have two major features, according to both of these definitions:

- The anomalies’ distribution deviates significantly from the data’s overall distribution.
- Standard data points make up the vast majority of the dataset. The anomalies make up a very small portion of the overall dataset.

The development of anomaly detection methods is dependent on these two factors. The second property, in particular, prevents the employment of common classification methods that depend on balanced datasets.

2.1.1 Types of Anomalies

Anomalies come in a variety of shapes and sizes. Anomalies can be divided into three categories:

1. **Point Anomalies** - A point anomaly occurs when a single point deviates dramatically from the rest of the data. A point anomaly is, for example, a large credit transaction that differs from other transactions.
2. **Collective Anomalies** - Individual points may or may not be anomalous, but a series of points may be. A bank customer, for example, withdraws \$500 from her account per weekday. Although withdrawing \$500 every now and then is common for the consumer, a series of withdrawals is unusual.
3. **Contextual Anomalies** - Some points can appear natural in one context but be identified as anomalous in another: In Germany, a daily temperature of 35 degrees Celsius is considered natural in the summer, but the same temperature in the winter is considered unusual.

Knowing ahead of time what kind of anomaly the data might contain helps the data analyst choose the best detection process. Some methods for detecting point anomalies fail to detect collective or contextual anomalies entirely (Braei and Wagner, 2020).

2.2 Anomaly Detection on Univariate Time Series

First, anomaly detection on univariate time series using deep learning approaches is investigated to gain insight on the used architecture and the overall training and detection process.

2.2.1 LSTM

Because of their ability to retain long term memory, Long Short Term Memory (LSTM) networks have been shown to be especially useful for learning sequences containing longer term patterns. Malhotra et al. (2015) model normal behavior with a predictor and then use the prediction errors to classify abnormal behavior. This is especially useful in real-world anomaly detection scenarios where instances of normal behavior are plentiful but instances of anomalous behavior are rare. For prediction, multiple time steps into the future are forecasted to ensure that the networks capture the temporal structure of the chain. As a result, each point in the series has multiple corresponding expected values made at various points in the past, resulting in multiple error values. The likelihood of normal behavior on the test data is calculated using the probability distribution of the errors produced when predicting on normal data. For this approach Malhotra et al. use a deep LSTM neural network. The proposed network architecture with two hidden layers is successfully applied on different univariate time series such as Electrocardiograms (ECG), a valve time series and a power demand dataset.

In their experiments, Chauhan and Vig (2015) used the same approach for different types of anomalies in ECGs such as premature ventricular contractions or atrial premature contractions.

Especially to mention is the training approach used in both papers. To train the LSTM based Recurrent Network the data was divided into four sets. a non-anomalous training set, a non-anomalous validation set, a mixture of anomalous and non-anomalous validation set and test set, also consisting of a anomalous and non-anomalous sequences.

2.2.2 CNN

The use of CNNs for time-series analysis has received interest in recent years. Munir et al. (2019) forecast time-series and identify anomalies based on the prediction error using a CNN architecture called deep-learning based anomaly detection method (DeepAnT). DeepAnT uses an architecture that is divided into two modules. The first module is called "Time Series Predictor". The "Time Series Predictor" consists of a CNN. As the name of the module indicates, the CNN is responsible for predicting the future time stamps of a given time series, whereas the "Anomaly Detector" module is responsible for tagging given data point as anomalous. Figure 2.1 represents the architecture of the CNN-based predictor module. It consists of two convolutional layers, each followed by a max-pooling layer. As the last layer, however, a fully connected layer, where all neurons are connected to all neurons of the previous layer, is used. The last is responsible for predicting the next time step. The number of output node, hereby, corresponds to the number of predicted time steps. One output node means only the next time step into the future is predicted, whereas three output nodes would imply a sequence of three data points are predicted.

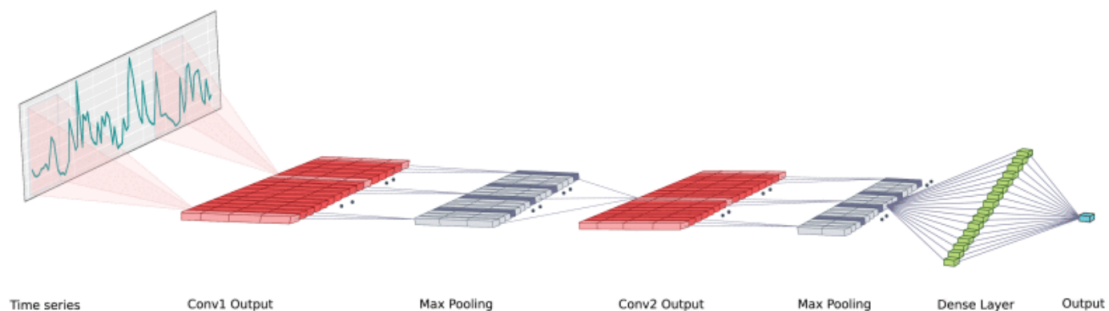


FIGURE 2.1: CNN ()

Once the next time steps are predicted, the values are then passed to the "Anomaly Detector". The detector module calculates the euclidian distance between the predicted and the actual data point. This measure of discrepancy is used as anomaly score. A high anomaly score indicates a significant anomaly at a given time step. For this module, a threshold based on the time series form must be specified. Most anomaly detection algorithms actually require such a threshold.

Ioffe and Szegedy suggest another regularization technique called Batch Normalization. Experiments in computer vision showed that Batch Normalization results in a higher learning rate, acts as an alternative for dropout layers and decreases the importance of careful parameter initialization. Therefore, we also implement a CNN architecture using Batch Normalization for univariate anomaly detection to evaluate its performance in anomaly detection.

2.2.3 Comparison

In an extensive study Braei and Wagner (2020) compared 20 different anomaly detection methods. The anomaly detection methods were divided into the three following categories.

- Statistical Methods

- Classical Machine Learning Methods
- Deep Learning Based Methods (Neural Networks)

Comparison of AUC

The methods were applied on data containing point, collective and contextual anomalies. In order to compare the different approaches, AUC-Values ¹ were used. The results showed that the statistical methods generally performed best on point and collective anomalies while deep learning approaches performed rather poorly. On a dataset that contained contextual anomalies, the situation reflected the exact opposite. Deep learning approaches clearly outperformed statistical methods. It was observed that deep learning approaches kept their ability to generalize while statistical methods overfitted on the data (Braei and Wagner, 2020).

Computation Time

The second parameter that was used to compare the different categories was training and inference time. Inference refers to the time used to classify the test data. Compared to statistical methods and classical machine learning, deep learning approaches once again performed rather poorly regarding training time. Looking at inference time deep learning approaches generally perform well, outperforming the other two categories. However, there are huge difference within the deep learning approaches. While CNNs have a very low inference time, and outperform most other algorithms, LSTMs have the highest inference time of all tested algorithms (Braei and Wagner, 2020).

2.3 Anomaly Detection on Multivariate Time Series

2.3.1 LSTM

2.3.2 CNN

Classification of Time Series Data using CNN

In their research project Zheng et al. (2014) tried to beat the state of the art classification algorithm for time series, which is the k-Nearest Neighbor algorithm(k-NN). k-NN has been empirically shown to be extremely difficult to beat. The typical problem of the k-NN algorithm, however, is its computation time. Zheng et al. proposed to use their own developed architecture, which is called Multi-Channel Deep CNN (MC-DCNN). Each channel, hereby represents a CNN with convolutional and pooling layers. Typically channels in CNN are used to extract features from the different spectra of pictures. A colored picture for example consists of three channels, red, green and blue. Each channel now works as feature extractor on just one color. This feature of CNN is now used in time series classification. Every channel learns features independently using a single dimension of the multivariate time series as input. Another difference to image classification is that multivariate time series classification uses multiple 1D subsequences rather than 2D image pixels as data. Because CNN only learn features, no classification can be done. In order to classify, a

¹An ROC curve (receiver operating characteristic curve) is a graph showing the performance of a classification model at all classification thresholds. The AUC measures the entire two-dimensional area underneath the entire ROC curve. See [ROC and AUC](#).

CNN architecture is combined with a Multilayer Perceptron (MLP) that uses fully connected layers. Figure 2.2 shows the just described architecture. It is important to note that this architecture does not predict the next time steps in the series but instead a given time series is directly classified. The classification is hereby for example used to classify the physical activity depending on the heartrate on is not used for anomaly detection. In order to use the proposed architecture for anomaly detection however, only the output layer has to be changed.

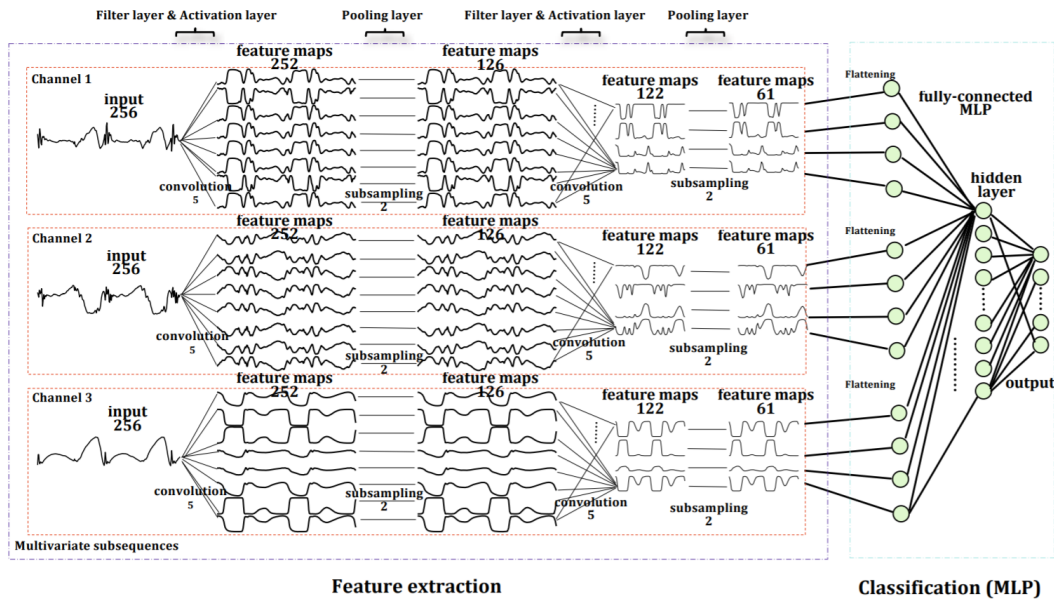


FIGURE 2.2: MC-DCNN ()

Zheng et al. state that the used architecture was superior to the k-NN algorithm regarding accuracy. Further, the experiments shows that deeper architecture are able to learn more robust high-level features. Further, the MC-DCNN architecture performs much faster than the k-NN algorithm, especially when a large dataset is present.

U-Nets for Anomaly Detection

Wen and Keyes (2019) use a special type CNN architecture to detect anomalies. The architecture used is called U-Net. A U-Net consists of so called encoding and decoding layers. The encoding layers work like a standard CNN whereas the decoding layers are used for upsampling. In short, the encoding layers extract the most important features of the time series and decoding layers are using these features to assemble a new time series of the same dimensions as the original one. This encoder-decoder-architecture is often referred to as autoencoder architecture. The main weakness of autoencoders is that in the encoding part through downsampling information is permanently lost. To prevent this information loss, U-Nets introduce so called skip channels also called skip connections. A skip connection, as the name implies, is one that connects an earlier part of the network to a later part of the network and transfers data. The idea is simple: skip channels bring back missing knowledge from some earlier layers so that the network can be properly contextualized. This architecture was proven successful when applied to segmentation of

neuronal structures in electron microscopic images in the original paper (Cicek et al., 2016). In order to handle multivariate time series U-Nets also make use multiple channels. Figure 2.3 shows the architecture of the above described U-Net.

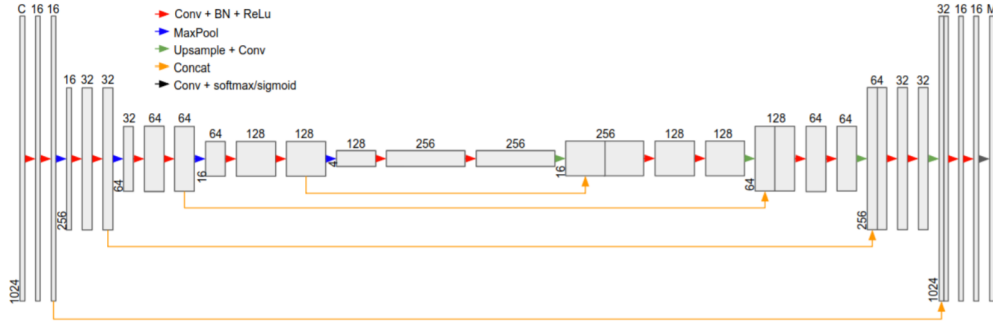


FIGURE 2.3: U-Net ()

Finally, the model tries to classify what kind of anomaly the multivariate time series contained e.g a seasonal anomaly (contextual) or a point anomaly. Depending on whether the anomaly classes are mutually exclusive or not either a sigmoid or softmax activation is used as last layer activation function.

The proposed U-Net was tested on four scenarios: a univariate task with sufficient data, a multivariate task with sufficient data, a univariate task with insufficient data and transfer learning, and a multivariate task with insufficient data and transfer learning.

For univariate task the dodgers loop sensor data was used. Ihler et al. is the first to introduce this data set2 (2006). It involves a 28-week time series of traffic on a ramp near Dodger Stadium with a 5-minute frequency. The goal is to spot unusual traffic patterns caused by sporting events. Out of 39 events, only three could not be detected. The missing detection were attributed to missing values in the data set. Missing values apparently also were the reason for some false positives.

For the multivariate task the gasoil heating loop data set was used. It contains 48 simulated control sequences for a gasoil plant heating loop that was hacked at one stage. There are 19 variables in all time series. A multivariate U-Net with 19 channels was trained. Out the 18, in the test present attacks, only one was missed. However, also 3 false alarms (false positives) were reported.

The tasks that included transfer learning are investigated further in section 2.5.

2.4 Parameter Settings for fair comparison

2.5 Transfer Learning

2.6 Research Gap

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