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Faculdade de Engenharia Mecânica

LEONARDO TADEU LIMA FRANCO

Título do seu Trabalho Acadêmico: dissertação de mestrado ou tese de doutorado

Campinas

Ano

Leonardo Tadeu Lima Franco

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Dissertação apresentada ao Instituto de Matemática, Estatística e Computação Científica da Universidade Estadual de Campinas como parte dos requisitos exigidos para a obtenção do título de Mestre em Matemática Aplicada e Computacional.

Orientadora: Auteliano Antunes dos Santos

Este exemplar corresponde à versão final da Dissertação defendida pela aluna Leonardo Tadeu Lima Franco e orientada pela Profa. Dra. Auteliano Antunes dos Santos.

Campinas

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Resumo

Segundo a **??**, 3.1-3.2), o resumo deve ressaltar o objetivo, o método, os resultados e as conclusões do documento. A ordem e a extensão destes itens dependem do tipo de resumo (informativo ou indicativo) e do tratamento que cada item recebe no documento original. O resumo deve ser precedido da referência do documento, com exceção do resumo inserido no próprio documento. (. . .) As palavras-chave devem figurar logo abaixo do resumo, antecedidas da expressão Palavras-chave:, separadas entre si por ponto e finalizadas também por ponto.

Palavras-chave: latex. abntex. editoração de texto.

Abstract

This is the english abstract.

Keywords: latex. abntex. text editoration.

List of Figures

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List of abbreviations and acronyms

UNICAMP	Universidade Estadual de Campinas
IMECC	Instituto de Matemática, Estatística e Computação Científica
LabCSD	Laboratório de Controle e Sistemas Dinâmicos
EPIFISMA	Laboratório de Epidemiologia e Fisiologia Matemática
LCP	Laboratório de Computação Paralela
LGC	Laboratório de Geofísica Computacional
LMDC	Laboratório de Matemática Discreta e Códigos
MiLAB	Laboratório de Tratamento Matemático de Imagens e Inteligência Computacional
LPOO	Laboratório de Pesquisa Operacional e Otimização
LEM	Laboratório de Ensino de Matemática
PAPMEM	Programa de Aperfeiçoamento para Professores de Matemática do Ensino Médio
OMU	Olimpíada de Matemática da Unicamp
CCPG	Comissão Central de Pós-Graduação
ABNT	Associação Brasileira de Normas Técnicas
abnTeX	ABsurdas Normas para TeX

List of symbols

$\mathbb{M}_{m\times n}(\mathbb{R})$	Conjunto das matrizes de ordem $m \times n$ com entradas reais
$\mathbb{R}^n_+$	Conjunto dos vetores x pertencentes a $\mathbb{R}^n$ que satisfazem $x \geqslant 0$
$\mathbb{R}^n_{++}$	Conjunto dos vetores x pertencentes a $\mathbb{R}^n$ que satisfazem $x > 0$
$\|\cdot\|$	Norma-p vetorial
$\|\|\|\cdot\|\|\|_p$	Norma-p matricial
$\mathbf{I}_n$	Matriz identidade de ordem $n \times n$
∇f	Gradiente da função f
∞	Infinito

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Contents

1 Introduction

Este documento e seu código-fonte são exemplos de referência de uso da classe abntex2 e do pacote abntex2cite. O documento exemplifica a elaboração de trabalho acadêmico (teses e dissertações) produzido conforme a **Informação CCPG/001/2015** (que trata das *Normas para impressão de teses/dissertações* da UNICAMP). Encorajamos o leitor a consultar a Informação CCPG/001/2015 (**??**) antes de iniciar as alterações neste documento e seu código-fonte.

A elaboração deste modelo teve como base uma customização do "Modelo Canônico de Trabalho Acadêmico com abnTEX2" (**??**) para que as normas presentes na Informação CCPG/001/2015 fossem respeitadas. O modelo original produzido pela equipe abnTEX2 cumpre as seguintes normas ABNT:

1. **ABNT NBR 14724:2011**: Informação e documentação - Trabalhos acadêmicos - Apresentação;
2. **ABNT NBR 10520:2002**: Informação e documentação - Citações;
3. **ABNT NBR 6034:2004**: Informação e documentação - Índice - Apresentação;
4. **ABNT NBR 6028:2003**: Informação e documentação - Resumo - Apresentação;
5. **ABNT NBR 6027:2012**: Informação e documentação - Sumário - Apresentação;
6. **ABNT NBR 6024:2012**: Informação e documentação - Numeração progressiva das seções de um documento - Apresentação
7. **ABNT NBR 6023:2002**: Informação e documentação - Referência - Elaboração.

Este documento deve ser utilizado como complemento dos manuais do abnTEX2 (**??????**) e da classe memoir (**??**).

A leitura do teor desde documento (tanto o PDF quando os arquivos que compõem seu código-fonte), bem como do arquivo LEIAME.txt é altamente recomendada para melhor entendimento da dinâmica de funcionamento da classe abntex2 e do pacote abntex2cite. Seus principais comandos e usos estão exemplificados no decorrer do texto, bem como outras informações relevantes para a escrita de seu trabalho acadêmico.

USAR https://www.tandfonline.com/doi/full/10.1080/00423114.2025.2483972 para pegar algumas informações interessantes.

2 Literature Review

2.1 Time Series Anomaly Detection

In recent years, rapid technological advancements have led to a significant increase in the volume of data collected and generated from diverse sources such as sensors, databases, and files (ATTOH-OKINE, 2017). This large volume of data is now commonly referred to as Big Data. A substantial portion of Big Data consists of data points collected in sequential time steps, also known as time series. Analyzing time series data presents a complex set of challenges (TSAI et al., 2015).

One of the most studied problems in this area is anomaly detection. It consists of identifying outliers or abnormal patterns within data and has a variety of applications, from financial systems and medical diagnosis to urban management and fault detection (BLáZQUEZ-GARCíA et al., 2021; CHOI et al., 2021; DARBAN et al., 2024; SAMARIYA; THAKKAR, 2021).

The following sections will dive deeper into what the concept of a time series is, what the different natures of anomalies in data are, and some of the models used to detect these anomalies.

2.1.1 Time Series

A time series (TS) can be defined as a set of points indexed sequentially over time and is often divided into univariate and multivariate. A univariate TS is a set of real values from a single variable that changes over time $\mathbf{X} = \{x_t\}$ for $t \in T$, where T is the total time. On the other hand, a multivariate TS is a set of real values from multiple variables that change over time, i.e., $\mathbf{X} = \{\mathbf{x}_t\}$ for $t \in T$, where $\mathbf{x}_t$ is a k-dimensional vector defined by $\mathbf{x}_t = (x_{1t}, ..., x_{kt})$ and each x_{it} is a univariate TS.

A subsequence of length $n \leqslant T$ can be defined as $\mathbf{S} = \{\mathbf{x}_{p:p+n}\}$ from the time series $\mathbf{X}$, where $p \in T$ and $p \leqslant T - n + 1$ (DARBAN et al., 2024; BLáZQUEZ-GARCíA et al., 2021).

Time series data exhibit dependencies that vary based on their type. In univariate time series, temporal dependency occurs when the value at time t, x_t, is influenced by its preceding values, $x_{p:t}$. In multivariate time series, in addition to temporal dependencies, there are spatial dependencies, representing the correlations between different variables within the same time step (DARBAN et al., 2024).

2.1.2 Time Series Anomalies

According to (GRUBBS, 1969) an anomaly can be defined as an outlier that deviates greatly from the general distribution of data. These outliers can be a single observation or a subsequence of the whole time series. Building on this, (BLáZQUEZ-GARCíA et al., 2021) divides anomalies into three main categories:

1. *Point Anomalies*: A point outlier can be defined as a single observation that deviates from the global behavior (global anomaly) or from the behavior of it's neighborhood (local anomaly). This type of anomaly can be identified using equation 2.1

$$|x_t - \hat{x}_t| > t \tag{2.1}$$

   where $\hat{x}_t$ is the expected result, x is the original data point and t is the threshold. If the difference is greater than the threshold t, then x_t is identified as an anomaly. Figure 1 shows an example of this anomaly, where O1 is a local outlier and O2 is a global anomaly.

2. *Subsequence Anomaly*: A subsequence outlier refers to a consecutive portion of points from the time series whose joint behavior is abnormal. It is important to note that each of these data points alone doesn't need to a point anomaly, but together they form an anomaly. Similarly to the point outliers, the subsequence outliers can be global or local. These anomalies can be identified by the equation (DARBAN et al., 2024):

$$diss\left(C, \hat{C}\right) > t \tag{2.2}$$

   where C is the the actual cycle or shape of the subsequence, $\hat{C}$ is the expected output, t is the threshold and $diss$ is a function that computes the dissimilarity between the two subsequences, such as the cosine similarity. Figure 2 shows an example of this, where O1 is a local anomaly and O2 is a global anomaly.

3. *Time Series Anomaly*: A time series anomaly is a entire timeseries that presents unusual behavior. Note that, this kind of anomaly can only be detected in multivariate time series. Figure 3 shows an example of this problem, where variable 4 behavior differs greatly from the other 3 variables.

(DARBAN et al., 2024) highlights another anomaly that can only occur in multivariate time series: the intermetric anomaly. An intermetric anomaly can be defined as an anomalous behavior in the correlation between two variables.

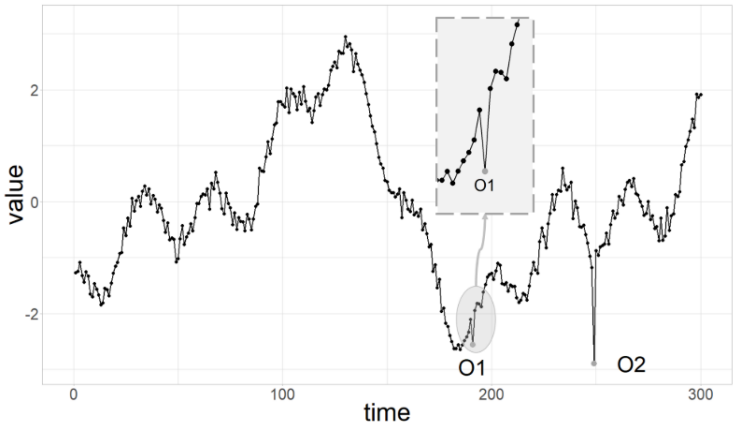


Figure 1 – (BLáZQUEZ-GARCíA et al., 2021)

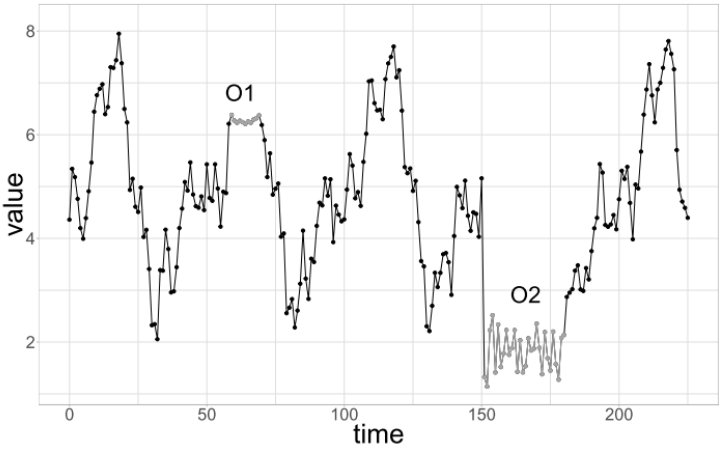


Figure 2 – (BLáZQUEZ-GARCíA et al., 2021)

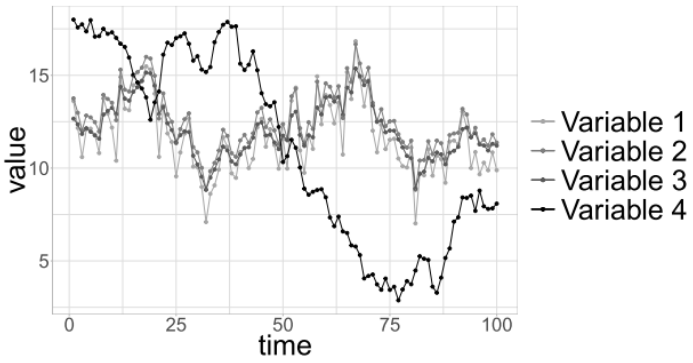


Figure 3 – (BLáZQUEZ-GARCíA et al., 2021)

2.2 Time Series Anomaly Detection Models

Since the 1960s, many models for anomaly detection have been proposed, ranging from statistical models to recent deep learning models. The common main idea

behind all of those is to identify low probability, i.e. low density, regions, classifying points in those areas as anomalies (SAMARIYA; THAKKAR, 2021).

Statistical models, for example, use statistical tests, like the χ^2 test, to identify abnormal points. Clustering-based models use cluster analysis to label anomalies, using, for example, the distance from the centroid of normal points or the number of points in a cluster. Distance-based models use the distance between the current time window and its neighborhood to classify anomalies. Density-based approaches use the density of the data points to find anomalies (DARBAN et al., 2024; SAMARIYA; THAKKAR, 2021). These methods described above are called traditional methods.

In recent years, with the increase of computing power, deep learning models have become increasingly prominent in anomaly detection. Unlike the traditional methods, the main advantage of deep learning models is that they are capable of identifying complex temporal and spatial correlations between variables, especially in larger multidimensional datasets, without the need for a labeled dataset (DARBAN et al., 2024; CHOI et al., 2021). (DARBAN et al., 2024) divides deep learning models into 3 main categories: forecasting-based models, reconstruction-based models, and representation-based models.

Forecasting-based models try to predict a future subsequence of the time series using historical data. These models learn the patterns and trends within data to anticipate what is expected to occur. Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTMs) are examples of this category. Anomalous values are detected if they deviate greatly from what the model predicts.

Reconstruction-based models attempt to recreate the input timeseries based on the values of past points or windows. These models use architectures like autoencoders (AE) and Generative Adversarial Networks (GANs). Anomalies are identified using the reconstruction error between the predicted series and the original series. The advantage of reconstruction-based models over forecasting ones is that they adapt better to rapid changes in a timeseries, which may cause it to become unpredictable. This happens because reconstruction models have access to the current timeseries data, which is not available in forecasting models (DARBAN et al., 2024). This better precision comes with a delay in the detection time of an anomaly, but, in general, these models are preferred over forecasting models.

Representation-based focus on learning meaningful representations of the data that can be used in downstream tasks, like anomaly detection. These models use advanced architectures like transformers and self-supervised learning to extract high-level features from the data. The learned representations are often used in conjunction with simpler models (e.g., clustering or density-based methods) to identify anomalies. The downside of these models is that they are computationally expensive to train, often needing a large amount of data.

An important point to highlight is that the majority of the models described above are unsupervised models. An unsupervised model is a model that can learn patterns from data without the need for a labeled dataset. This flexibility is desired because of the inherently unlabeled nature of historical data and the unpredictability of anomalies, which makes it harder to define an anomaly, especially if anomalies are rare. In this work, the focus will be on unsupervised reconstruction models.

2.3 Basics of Deep Learning Models

Before diving deeper into anomaly detection models, the fundamental concepts of deep learning will be presented first. This preliminary discussion will provide the necessary context and theoretical basis for the subsequent exploration of anomaly detection methodologies.

2.3.1 Neural Networks

Neural networks are the most basic structure in deep learning. It is inspired by the way the human brain works (AGATONOVIC-KUSTRIN; BERESFORD, 2000; ALZUBAIDI et al., 2021). These networks are composed of thousands, or even millions, of interconnected units called perceptrons, which mimic the behavior of biological neurons. In a neural network, these perceptrons are arranged into multiple layers, as shown in Figure 4(a). In this illustration, each circle represents a single perceptron.

The neural network is divided into three main components:

- The input layer: this layers receives raw data that will be precessed;
- The hidden layers: positioned between the input and output layers, these intermediate layers perform feature extraction;
- The output layer: this layer provides predictions or classifications

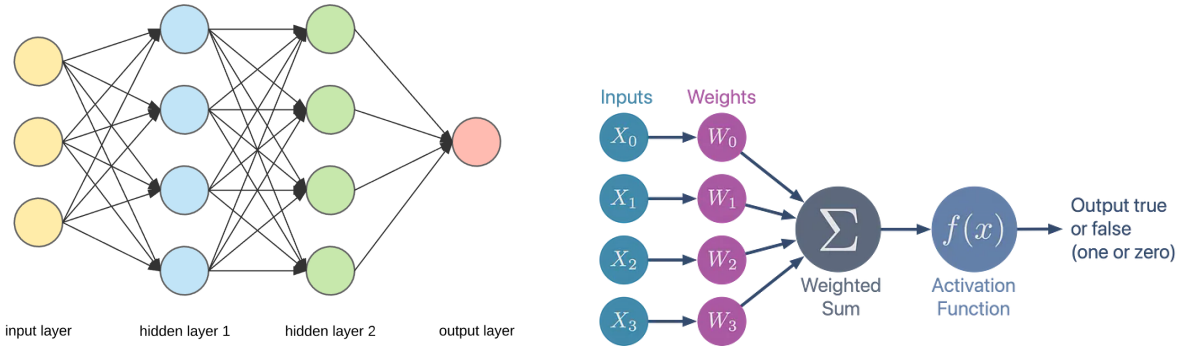
Each perceptron in a neural network processes input data linearly using the dot product. Given, them, an input array $\mathbf{x}$, the perceptron computes the output by multiplying $\mathbf{x}$ with an array of weights $\mathbf{w}$ and adding a bias b, producing a scalar output o (GURNEY, 1997):

$$o = \sum_i w_i x_i + b \tag{2.3}$$

The weights and biases are learned and iteratively updated during the training process such that they minimize the errors.

However, in its basic form, a perceptron can only solve linearly separable problems. To address this limitation, modern perceptrons include an additional element:

the activation function. An activation function introduces non-linearity into the model, enabling it to solve complex, non-linear problems (ROTH, 2016).For reasons that will be explained later, it is common to choose differentiable activation functions. Common activation functions include the Rectified Linear Unit (ReLU) and the hyperbolic tangent (tanh). The general structure of a perceptron, including the activation function, is illustrated in Figure 4(b).



((a)) (P., 2025) ((b)) (WEAVER, 2024)

Figure 4 – Caption

As mentioned earlier, the weights and biases of the perceptrons are adjusted and optimized during the training phase of a neural network. This optimization process involves a method called backpropagation, which is essential for minimizing the error in predictions. Backpropagation, discussed in detail in Section 2.3.2, leverages the gradient descent algorithm to iteratively update the network's parameters, ensuring improved accuracy over successive training iterations.

2.3.2 Backpropagation

During the training phase of a neural network, its weights and biases are systematically optimized to minimize the error. This iterative process comprises two key subprocesses: a forward pass followed by a backward pass. In a forward pass, the inputs are passed through the network and the outputs are calculated. Then, given an expected output, an error is computed using a function called the loss function. The backward pass, then, uses this error to update the weights and biases of the neural network, making it better at making right predictions. This process continues until the error is small enough.

The process of propagating the error back through the network during the backward pass is referred to as backpropagation. It can be broken down into four primary steps (CILIMKOVIC, 2015):

1. Feed foward the inputs;
2. Backpropagation to the output layer;

3. Backpropagation to the hidden layers;

4. Weights updates.

The first step is just feeding forward the inputs $\mathbf{x}$ through the network and obtaining the outputs $\mathbf{o}$. Then, a loss is computed using the loss function $\mathbf{L}$. There are a variety of loss functions, an example being the Mean Squared Error (MSE):

$$\mathbf{L} = \frac{1}{N}\sum_i (y_i - o_i)^2 \tag{2.4}$$

where y_i is the desired output and o_i is the network output. To backpropagate the error, the algorithm computes gradients of the loss function with respect to the parameters of the neural network. This is done using the chain rule twice (ROTH, 2016):

$$\frac{\partial \mathbf{L}}{\partial w_{ij}} = \frac{\partial \mathbf{L}}{\partial o_j}\frac{\partial o_j}{\partial net_j}\frac{\partial net_j}{\partial w_{ij}} \tag{2.5}$$

where w_{ij} is the i-th weight of the j-th perceptron, net_j is the result of the dot product before applying the activation function, i.e.,

$$net_j = \sum_i w_{ij}x_j \tag{2.6}$$

with x_j being the input, and o_j the perceptron output, i.e.,

$$o_j = \varphi(net_j) \tag{2.7}$$

where φ is the activation function of the perceptron. For this reason, it is necessary that the activation function is a differentiable function.

To update the weights, the algorithm computes, then, the incremental Δw_{ij} using:

$$\Delta w_{ij} = -\eta\delta_j x_{ij} \tag{2.8}$$

where η is a small positive number known as the learning rate, $\delta_j = \dfrac{\partial \mathbf{L}}{\partial net_j}$ and x_{ij} are the inputs of the j-th perceptron, and, thus, update the weights as:

$$w_{ij} \leftarrow w_{ij} + \Delta w_{ij} \tag{2.9}$$

For a full demonstration of these formulas, check Appendix A.

Despite its effectiveness, the classical backpropagation algorithm has some problems associated with its convergence. For example, if the learning rate is too small, the convergence is very slow and can converge to a local minimum; on the other hand, if it is too large, the algorithm can diverge (RUDER, 2016). Several modifications to the original algorithm have been proposed, like in (QIAN, 1999), (TIELEMAN, 2012) and (KINGMA; BA, 2017), but the contents of these works are outside the scope of this thesis.

2.3.3 Convolutional Neural Networks

Convolutional neural networks (CNN) achieved great popularity in modern machine learning, gaining large popularity with the (KRIZHEVSKY; SUTSKEVER; HINTON, 2012) paper. In this work, the authors proposed a deep CNN that won the ImageNet LSVRC-2010 contest, outperforming second place by a large margin.

A CNN, similarly to the neural network, was inspired by the biological neurons, but, different from the conventional neural network, where all the neurons are connected and interact with all neurons in adjacent layers, the CNN employs a sparse architecture, i.e., the neurons are connected only to a local region of the input. This sparsity reduces the amount of training parameters, which reduces the computational cost and speeds up the training process (ALZUBAIDI et al., 2021; LI et al., 2022).

CNNs are widely used in computer vision to process and analyze 2D images and are used to solve a variety of image-related problems, like classification and object detection. While this section focuses on explaining CNN concepts with the assumption of a 2D input, it is important to note that the principles discussed are equally applicable to 1D inputs, like in a timeseries.

The basic block of a CNN is the convolution operation. A convolution can be defined as the dot product between an input x of shape (m, m, r), where m is the height, which is the same as the width, and r is the depth, also called the channel number, and k convolutional filters, called kernels. A kernel is a grid of weights, with shape (n, n, q), where $n < m$ and $q \leqslant r$, that convolves with the input, producing, each, an output of size $(m - n - 1)$, called the feature maps (ALZUBAIDI et al., 2021). These kernels compute the pass value similarly to the

$$h^k = f\left(W^k * x + b_k\right) \tag{2.10}$$

where W^k is the vector of weights from the kernel, f is an activation function, and b^k is the bias. Figure 5 shows an example of this operation between a 2D binary matrix and a 3×3 kernel.

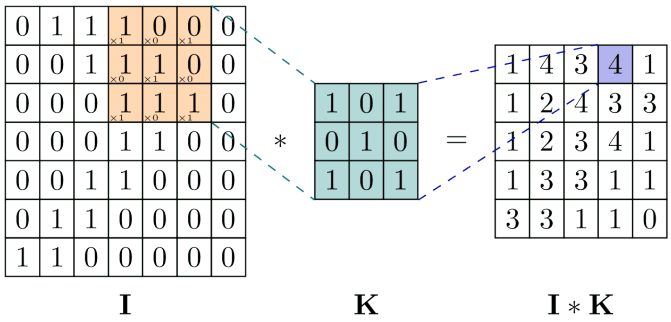


Figure 5 – (RIEBESELL, 2022)

In addition to the convolution operation, there are two other important parameters in convolutional neural networks: the padding and the stride. Their main function is to control the output size of the convolution, helping to maintain the spatial characteristics of the input.

The padding is the process of adding additional rows and columns around the border of the input matrix, typically filled with zeros, a process known as zero padding. Without the padding, a convolution with a kernel of size $n \times n$ reduces the output size by $n-1$ in each spatial dimension. This would cause a rapid decrease in the size of the features, that would force the use of small kernels (GOODFELLOW; BENGIO; COURVILLE, 2018).

Stride, on the other hand, controls how the kernel moves across the input matrix, by skipping some of the elements from it. In a stride 1 convolution, the kernel shifts one unit at a time, covering all the positions. In a stride 2 convolution, the kernel would shift 2 elements each time, which causes the kernel to convolve with every other element. In general, a stride of size s means that the kernel will only convolve every s elements. This is done primarily to reduce computational cost, at the expense of extracting the features less finely (GOODFELLOW; BENGIO; COURVILLE, 2018).

Now with these two additional operations, the output size can be computed using the formula:

$$O = \left\lfloor \frac{I + 2 \cdot p - k}{s} \right\rfloor + 1 \tag{2.11}$$

where O is the output size, I is the input size, p is the padding, k is the kernel size, and s is the stride.

Another important feature that is widely used in CNNs is the pooling layer. Pooling layers are used to further reduce the spatial dimension of the feature map by replacing the output value of the convolution operation with a local summary statistic, which helps the model to develop representations that are invariant to small translations (GOODFELLOW; BENGIO; COURVILLE, 2018).

One of the most widely used types is max pooling, which selects the maximum value within a local neighborhood, as shown in Figure 6. Other common pooling methods include average pooling, which computes the mean of the values within the region, and weighted average pooling, where each value contributes proportionally based on predefined weights.

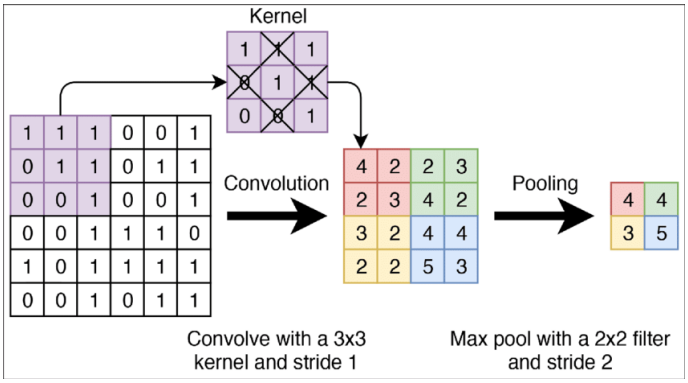


Figure 6 – (VAART; LAMBERS, 2019)

2.4 Recurrent Neural Networks

Recurrent Neural Networks (RNNs) are a type of artificial neural network specifically designed to work with sequential data, such as time series, speech recognition, text generation, and language modeling (SCHMIDT, 2019; FANG; CHEN; XUE, 2021; ALZUBAIDI et al., 2021). The main difference between an RNN and the networks discussed in Sections 2.3.1 and 2.3.3 is how data is processed inside the RNN. In the MLP and the CNN networks, it is assumed that each input is independent from each other, which can be a valid assumption when dealing with images, but might be a severe limitation when dealing with sequential data, like weather data, where, for example, the current temperature depends on the last few measurements.

RNNs deal with this kind of problem by introducing a cycle in their architecture allows information to persist across time steps (SCHMIDT, 2019), as shown in Figure 7. The key idea is to add a hidden-to-hidden weight matrix $\boldsymbol{W}_{hh}$ that carries information from the previous hidden state $\boldsymbol{H}_{t-1}$ in the computation of the current hidden state $\boldsymbol{H}_t$.

The current hidden state can be computed using Equation 2.12:

$$\boldsymbol{H}_t = \phi(\boldsymbol{X}_t \boldsymbol{W}_{xh} + \boldsymbol{H}_{t-1} \boldsymbol{W}_{hh} + \boldsymbol{b}_h) \tag{2.12}$$

where $\boldsymbol{X}_t$ is the input vector, $\boldsymbol{W}_{xh}$ is the input-to-hidden weight matrix, $\boldsymbol{b}_h$ is the bias, and ϕ is an activation function.

An important observation is that it is not necessary to explicitly include all previous hidden states, from $\boldsymbol{H}_0$ up to $\boldsymbol{H}_{t-2}$, when computing $\boldsymbol{H}_t$. This is because, at each iteration, the RNN updates $\boldsymbol{H}_t$ by combining the input $\boldsymbol{X}_t$ with the previous hidden state $\boldsymbol{H}_{t-1}$, which is the result of the computation between $\boldsymbol{X}_{t-1}$ and $\boldsymbol{H}_{t-2}$, and so on recursively. This way, the network can keep information about the previous time steps when computing the next one.

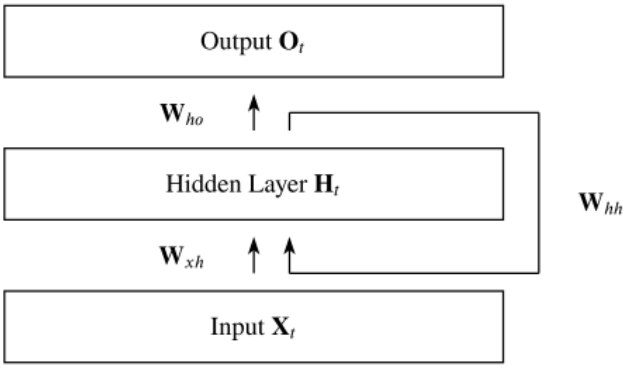


Figure 7 – Adapted from (SCHMIDT, 2019)

The main problem in the original RNN architecture arises during the training phase, specifically when computing gradients for weight updates. As gradients are propagated backward through time, a series of repeated multiplications occurs. If these values are greater than 1, the gradients can grow exponentially, causing the network weights to change abruptly fast. Conversely, if the values are less than 1, the gradients decay exponentially, which causes the gradient to vanish (KOLEN; KREMER, 2001; GLOROT; BENGIO, 2010). The vanishing gradient then causes the network to forget information from the initial time steps, which makes it difficult for RNNs to learn long-term dependencies in data.

This inherent problem motivated the introduction of more complex architectures, such as the LSTM networks. These networks will be explained in more detail in 2.5, but they mitigate the vanishing gradient problem, which caused the original RNNs to be barely used in today's research (FANG; CHEN; XUE, 2021; GAO et al., 2019).

2.5 LSTM

Long Short-Term Memory (LSTM) units were introduced by Hochreiter and Schmidhuber in 1997 (HOCHREITER; SCHMIDHUBER, 1997) and were specifically designed to deal with the vanishing gradient problem. Differently from vanilla RNNs, which struggle to retain information over long sequences, LSTM cells are specifically designed to capture long-term dependencies by preserving information across many time steps (AL-SELWI et al., 2024; SCHMIDT, 2019).

The core idea behind the LSTM architecture lies in its gating mechanism, which regulates the flow of information through the cell. This mechanism is composed of three gates: the forget gate, the input gate, and the output gate, shown in Figure 8. Each gate uses a sigmoid activation function, producing values between 0 and 1 to determine how much information should pass through (SCHMIDT, 2019).

- The forget gate decides which parts of the previous cell state should be discarded, allowing the network to "forget" irrelevant or outdated information.
- The input gate determines which portions of the new input information should be added to the cell state.
- The output gate controls which parts of the internal cell state are exposed as the output hidden state at the current time step.

The forget and input gates are responsible for updating the cell state, which acts as an internal memory, carrying forward important information throughout the sequence. The output gate, meanwhile, regulates how much of the updated cell state should influence the hidden state output. Through this mechanism, LSTMs are able to maintain and regulate long-term information flow (AL-SELWI et al., 2024).

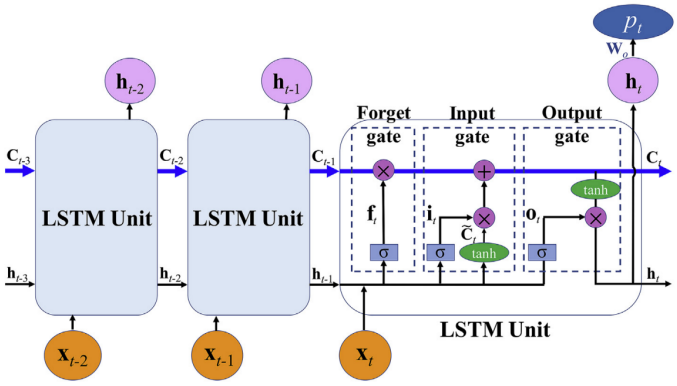


Figure 8 – Adapted from (WEI et al., 2021)

Using the same notation from Section 2.4 one can compute:

$$\boldsymbol{O}_t = \sigma\left(\boldsymbol{X}_t \boldsymbol{W}_{xo} + \boldsymbol{H}_{t-1} \boldsymbol{W}_{ho} + \boldsymbol{b}_o\right) \tag{2.13}$$

$$\boldsymbol{I}_t = \sigma\left(\boldsymbol{X}_t \boldsymbol{W}_{xi} + \boldsymbol{H}_{t-1} \boldsymbol{W}_{hi} + \boldsymbol{b}_i\right) \tag{2.14}$$

$$\boldsymbol{F}_t = \sigma\left(\boldsymbol{X}_t \boldsymbol{W}_{xf} + \boldsymbol{H}_{t-1} \boldsymbol{W}_{hf} + \boldsymbol{b}_f\right) \tag{2.15}$$

where $\boldsymbol{O}_t$, $\boldsymbol{I}_t$, and $\boldsymbol{F}_t$ are the inputs for the output gate, the input gate, and the forget gate, respectively. After this computation, the LSTM unit computes the candidate memory cell $\tilde{\boldsymbol{C}}_t$, which represents the candidate information that could be added to the cell state, as:

$$\tilde{\boldsymbol{C}}_t = \tanh\left(\boldsymbol{X}_t \boldsymbol{W}_{xc} + \boldsymbol{H}_{t-1} \boldsymbol{W}_{hc} + \boldsymbol{b}_c\right) \tag{2.16}$$

After that, the LSTM introduces the previous memory content $\boldsymbol{C}_{t-1}$, which, together with the other gates, controls how much of the old memory information will be retained in the new memory state $\boldsymbol{C}_t$, which can be computed using:

$$\boldsymbol{C}_t = \boldsymbol{F}_t \otimes \boldsymbol{C}_{t-1} + \boldsymbol{I}_t \otimes \tilde{\boldsymbol{C}}_t \tag{2.17}$$

where $\otimes$ denotes the element-wise multiplication. Finally, the LSTM unit computes the hidden state $\boldsymbol{H}_t$ as:

$$\boldsymbol{H}_t = \boldsymbol{O}_t \otimes \tanh(\boldsymbol{C}_t) \tag{2.18}$$

It is important to notice the hidden state $\boldsymbol{H}_t$ is used as the output of the LSTM cell and, together with the memory state $\boldsymbol{C}_t$, is used in the computation of the next time step.

2.6 Attention

Attention is an important concept in deep learning that was first introduced by (BAHDANAU; CHO; BENGIO, 2016) in a machine translation problem and gained widespread popularity with the famous paper "Attention Is All You Need" proposed by (VASWANI et al., 2023), where the authors proposed the transformer architecture. Inspired by the human attention of selectively focusing on relevant information, attention mechanisms enable neural networks to assign different weights to different parts of the input, allowing the model to concentrate on the most important elements of the data. This selective focus not only improves the model's interpretability but also makes it possible to handle large amounts of information more efficiently, reducing computational overhead (NIU; ZHONG; YU, 2021).

The attention mechanism works by taking a vector of features $\boldsymbol{F}$, which are obtained after the input data $\boldsymbol{X}$ is passed through a feature extraction model to extract the feature vectors $\boldsymbol{f}_1$, to $\boldsymbol{f}_n$. This feature extractor can vary depending on the task and, in the case of time series analysis, for example, it could be an encoder composed of CNNs, MLPs, or LSTMs, that produces the latent representations $\boldsymbol{f}_1$ to $\boldsymbol{f}_n$ (BRAUWERS; FRASINCAR, 2023).

From the feature vectors $\boldsymbol{F}$ the model then extracts the key and value vectors $\boldsymbol{K}$ and $\boldsymbol{V}$, respectively. These vectors are usually obtained through a linear transformation of $\boldsymbol{F}$ using the weight matrix $\boldsymbol{W}_K$ and $\boldsymbol{W}_V$.

After that, the model introduces a query vector $\boldsymbol{Q}$, which is a task-specific vector that guides the attention mechanism to focus on the most important vectors (BRAUWERS; FRASINCAR, 2023; NIU; ZHONG; YU, 2021). From the query and key vectors, the model then computes the energy score $\boldsymbol{e}$ using a score function f:

$$\boldsymbol{e} = f(\boldsymbol{Q}, \boldsymbol{K}) \tag{2.19}$$

where f can be a variety of functions, such as the scaled dot product (VASWANI et al., 2023):

$$f(\boldsymbol{Q}, \boldsymbol{K}) = \frac{\boldsymbol{Q}^T \boldsymbol{K}}{\sqrt{d_k}} \tag{2.20}$$

The energy scores $\boldsymbol{e}$ are then mapped to the attention weights $\boldsymbol{\alpha}$ using an attention distribution function g, usually the softmax function (NIU; ZHONG; YU, 2021):

$$\boldsymbol{\alpha} = \mathrm{g}(\boldsymbol{e}) \tag{2.21}$$

Using the attention weights $\boldsymbol{\alpha}$ and the value vector $\boldsymbol{V}$, the model computes the context vector $\boldsymbol{c}$ using:

$$\boldsymbol{c} = \sum_{l=1}^{n} \alpha_l \boldsymbol{V}_l \tag{2.22}$$

where $\alpha_l \in \mathrm{R}^1$ is the weight of the l-th vector. Figure 9 shows the architecture of the attention model.

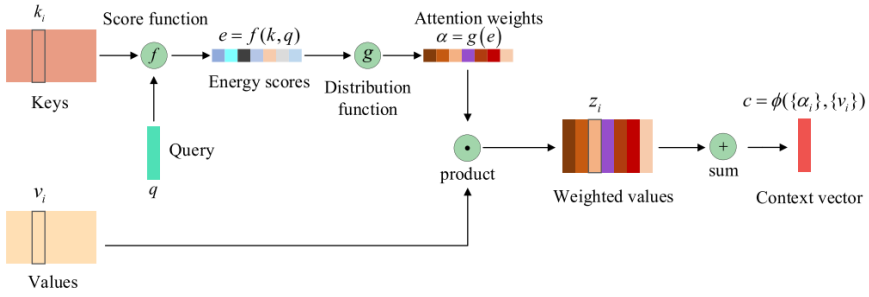


Figure 9 – (NIU; ZHONG; YU, 2021)

2.7 Transformers

2.8 Reconstruction-Based Models

Reconstruction-based models are a class of machine learning models that are designed to learn the intrinsic correlations in data by trying to reconstruct the original input signal. Differently from forecasting-based approaches, which attempt to predict future values, reconstruction-based models focus on accurately recreating the current input. This approach makes them great for anomaly detection, often outperforming forecasting-based models because they have access to the current time series data, which helps them to be more stable to rapidly changing time series. However, this advantage comes with a trade-off because they introduce a delay in the detection of anomalies as they rely on reconstruction error analysis. (DARBAN et al., 2024).

The main idea behind these networks is to train them to accurately reconstruct normal data, which is presumed to be the majority of the available data. This is usually done by minimizing a reconstruction loss, such as the Mean Squared Error (MSE), during the training phase.

During the test phase, the model encounters anomalous data, which it has not been trained to reconstruct, causing the reconstruction error to increase greatly compared

to the error of normal data, as the model fails to reconstruct abnormal patterns. This way, an anomaly can be identified by thresholding the reconstruction error. Inputs with low reconstruction error will be classified as normal, and inputs with reconstruction error greater than the threshold will be classified as anomalous.

There are a variety os reconstructions-based models, in Sections **??** and TODO: terminar de escrever sobre os modelos, escrever sobre defeitos, escrever sobre remocao do efeito de velocidade

2.9 Railway Components

The railway track consists of different interdependent components that are divided into two categories: the superstructure and the substructure. The former comprises the rails, fastenings, and sleepers, while the latter consists of the ballast, sub-ballast, and subgrade (KAEWUNRUEN[1]; REMENNIKOV[1], 2008), as shown in Figure ???. These two structures are separated by the sleeper-ballast interface and are essential for ensuring a safe and cost-effective transportation system capable of guiding vehicles and transmitting loads to the subgrade (ATTOH-OKINE, 2017).

INSERIR FIGURA AQUI

2.10 Railway Track Irregularities

Railway track defects

2.11 Assessing Railway Track Condition

Maintaining railway tracks in good condition is crucial to ensure safe and comfortable operations of trains (TSUNASHIMA, 2019; GHIASI et al., 2025). This maintenance is achieved through continuous monitoring of track conditions and the detection of irregularities. There are now two main methods to assess track quality: using track geometry cars (TGC) to directly measure the physical geometry of the track, and monitoring the dynamic response of the train using instrumented railway vehicles (IRV) equipped with onboard sensors capable of measuring the dynamics of the system (PIRES et al., 2024).

TGCs are equipped with sophisticated systems that directly measure the geometry of the track, that can be later compared to regulatory standards limits to identify parts of the track that need maintenance. However, this method has several drawbacks (PIRES et al., 2024; GHIASI et al., 2025; ONO et al., 2023):

- Operational disruption: the operation of the railway track needs to be disrupted during the TGC inspection, which can halt operations for several hours depending on the length of the track being measured;
- Operational high cost: the sophisticated equipment and logistics make TGC operation costly, which limits their frequent use;
- Low inspection frequency: normally, the TGC measures the condition of the track monthly, due to its high cost, which is a problem if a fault appears between inspections.

To overcome the limitations in TCGs, an alternative approach was developed using IRVs equipped with sensors that measure the vehicle's dynamic response due to track excitations. The underlying principle behind IRVs is that the vehicle's vibrations are deeply correlated to track excitations (PIRES et al., 2024; TSUNASHIMA, 2019), and an irregularity in the track will cause an anomalous dynamic response from the vehicle, which can be identified in the sensors' readings.

Using IRVs instead of the TCGs has several advantages, such as (PIRES et al., 2024; GHIASI et al., 2025; ONO et al., 2023):

- No disruptions: the operation is not halted during the measurements, since data can be collected during normal train services, which reduces the costs with logistics;
- Real time data collection: data is collected in real time, which speeds up possible defect detections;
- High frequency of inspections: Since the measurements are taken directly from in-service trains, IRVs enable near-continuous monitoring of track conditions, greatly increasing the inspection frequency.

Despite that, it is important to highlight that data collection using IRVs also comes with some drawbacks, such as (PIRES et al., 2024; GHIASI et al., 2025):

- High amount of data: the amount of data collected during IRV operation can be huge. This data needs to be carefully processed to obtain good quality data;
- Domain problem: different operations conditions, such as the wagon mass or velocity, can affect the dynamic response of the vehicle, so data collected from a one part of the track can be inherently different from another part;
- Correlation: since the measurements are done indirectly, they need to be correlated to the track condition, which can be a complex task that often needs the use of deep learning models;

- Data imbalance: since fault measurements are much more uncommon than normal measurements, the machine learning model needs to deal with class imbalance.

2.12 Velocity Effect on Train Dynamics

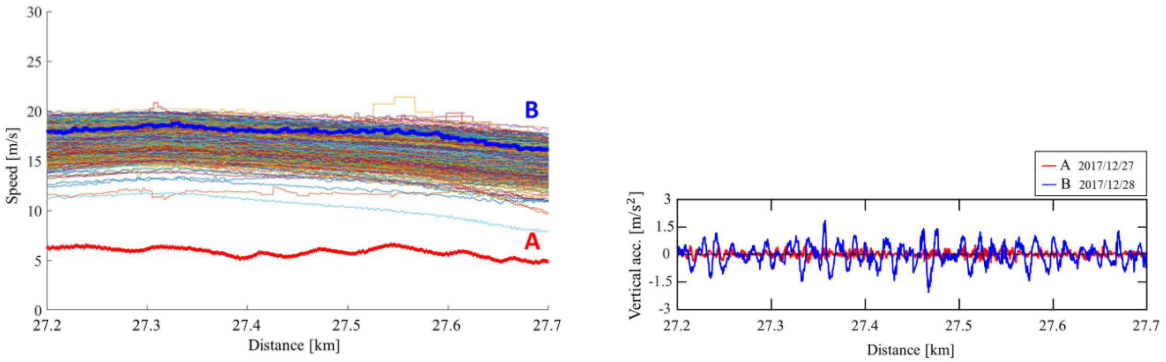
Train vibration measurements are strongly correlated to the velocity at which these measurements took place. As the wagon moves along the track, changes in velocity can alter the vibration responses measured by onboard sensors. At lower speeds, the dynamic response of the train to the track excitations tends to produce lower acceleration values than expected, while, for the same part of the track, higher velocities generate higher values of acceleration measured (ONO et al., 2023). Figure 10 shows this difference in measurement found by (ONO et al., 2023).

In Figure 10(a), the authors highlight two distinct velocity profiles labeled A and B, where the speed ratio between B and A is approximately 3. This difference in speed causes a significant change in the measured signal, as shown in Figure 10(b), where the velocity profile B generated bigger acceleration measures than A despite them traversing the same part of the track.

To address this velocity-induced distortion, the authors propose two different correction methods. The first method involves using the Mahalanobis distance to distinguish outliers from normal data. After that, the authors fitted a linear regression to normal data to predict the expected acceleration given the speed. The measurements are then normalized by dividing them by their predicted values.

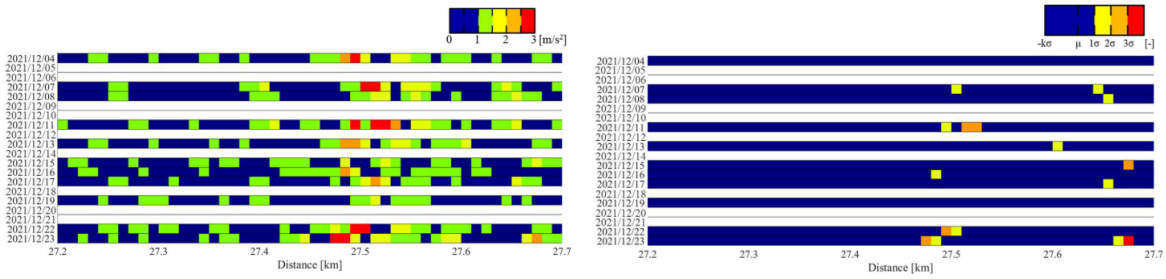
In the second method, the authors employed a Gaussian process regression to model the behavior of acceleration and speed, obtaining a regression that mapped the velocity to the expected acceleration. Similarly, they normalized the measurements by their respective predictions.

Both methods proved to be effective in mitigating the velocity effect, which reduced the number of false positives in anomaly detection, as shown in Figure 11.



((a)) (ONO et al., 2023) ((b)) (ONO et al., 2023)

Figure 10 – Caption



((a)) (ONO et al., 2023) ((b)) (ONO et al., 2023)

Figure 11 – Caption

Another example demonstrating the impact of the velocity on measured acceleration is presented in (BALOUCHI; BEVAN; FORMSTON, 2021). In this work, the authors utilized the VAMPIRE vehicle dynamics simulation software to model a vehicle operating in a measured track geometry at a variety of speeds. The simulated results were then compared to the actual car body vibration measurements recorded over the same section of the track. The results are shown in Figure 12, where the continuous colored lines are the simulation results, blue circles represent the maximum acceleration found in the simulation, and the dashed lines are the car body measurements.

The authors fitted two models to the maximum simulated accelerations: a linear regression, the green line in Figure 12 and an exponential model, the purple curve in Figure 12, to the maximum simulation acceleration, selecting the exponential model as it has a bigger R^2 value. They then argue that at lower speeds, the acceleration response does not yield a good level of confidence to differentiate if the quality of the track is good or bad, and so a normalization similar to (ONO et al., 2023) is necessary.

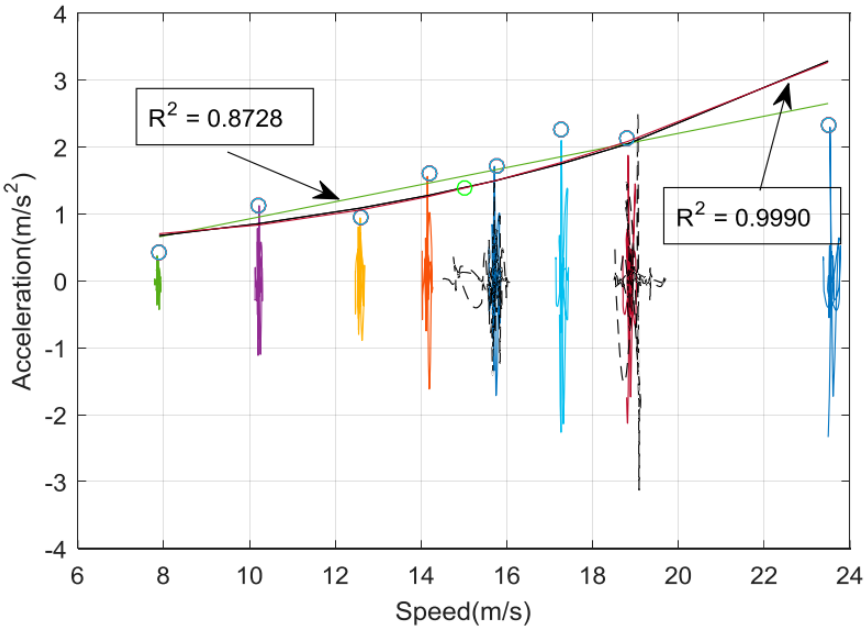


Figure 12 – (BALOUCHI; BEVAN; FORMSTON, 2021)

2.13 Assessing Track Quality from Acceleration Data

As stated in Section 2.11, continuous measurements of track irregularities are an important factor in ensuring safety and comfort during railway operations. Traditionally, TGCs were used to assess track irregularities by directly measuring the track geometry. However, due to their high cost, constant inspection of the railway is not possible.

An alternative to this approach is to use an IRV equipped with sensors that can measure the dynamic response of the vehicle due to track excitations. Normally, in this setup, accelerometers are mounted on various one or more components of the train, such as the axlebox, the bogie, or the car body, depending on the objective of the measurement and the maintenance costs of the sensors (TSUNASHIMA; YAGURA, 2024; SANSINENA; RODRíGUEZ-ARANA; ARRIZABALAGA, 2025).

In (SANSINENA; RODRíGUEZ-ARANA; ARRIZABALAGA, 2025) authors presented a review of research papers that proposed methods for estimating track irregularities using acceleration data. They divided the methods into three main categories:

- Model-driven methods;
- Data-driven methods;
- Hybrid methods.

In model-driven methods, a mathematical representation of the dynamic system is developed and validated on real data. Once the model accurately represents the system

dynamics, the problem is inverted to estimate track irregularities from the measured acceleration data. The main advantage in model-driven methods is that they don't require a large amount of data to be designed, as they're based on expert knowledge.

For instance, in (De Rosa; ALFI; BRUNI, 2019) the authors used a 3D multibody model that was previously validated to measure the yaw and roll motions of the vehicle. Based on simulation data, they applied three reconstruction techniques, the Kalman filter, the Unknown Input Observer (UIO) and the Frequency Response Function (FRF), to reconstruct the lateral irregularities and the cross alignment. The performance of these methods was compared using two evaluation metrics, but the detailed results are out of the scope of this thesis. They then tested the FRF method on real measured data, which included lateral and vertical accelerations recorded at the axle-boxes, bogies, and car body, obtaining the reconstruction shown in Figure 13. The authors argue that although some similarity between the reconstructed and the original irregularities can be seen, the method did not produce satisfactory results. They justify that this deviation is caused by non-linear effects they didn't consider, but these deviations can occur because of the lack of robustness of the method to real-world noise in data, which is a common problem when dealing with simpler reconstruction methods.

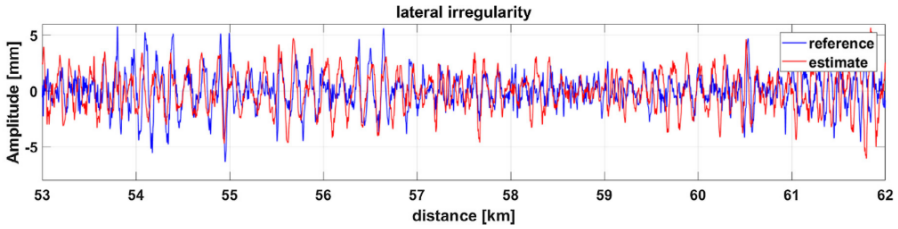


Figure 13 – (De Rosa; ALFI; BRUNI, 2019)

Data-driven methods, on the other hand, do not consider a mathematical model of the system, relying only on data processing to reconstruct or identify the irregularities. These methods typically utilize traditional machine learning algorithms or, more recently, deep learning architectures. Such approaches are generally more robust when dealing with real-world data, as they can learn from noisy and complex signals. This robustness, however, comes with a price, as they need a larger amount of data to be trained, especially in the case of deep learning (SANSINENA; RODRíGUEZ-ARANA; ARRIZABALAGA, 2025).

In (TSUNASHIMA; YAGURA, 2024) the authors propose a method of estimating railway track irregularities from car body vibration data. They first created a multibody simulation in SIMPACK. After that, they generated 12 different track irregularities, ranging from a good condition to a degraded condition, using FRA PSD formula and converted the generated profiles into 10 meters long track irregularity sections using the 10 m-chord versine method. This transformation is shown in Figure 14.

Using these irregularity profiles, they ran simulations over a 1000 meters track at speeds in the range of 40 to 80 km/h, varying the velocity in a 10 km/h interval. For each combination of track profile and speed, they collected the vertical and lateral acceleration as well as the roll rate of the carbody. Similarly to the irregularity profiles, a downsample was also applied to the data taking the maximum vibration measured in the 10 meters section, as shown in Figure 14. From this process, they obtained a dataset that correlates the maximum vibration of the carbody to the track irregularities for varying speeds and then applied a Gaussian Process Regressor (GPR) that was able to predict the irregularity from the vibration for a certain vehicle speed, as illustrated in Figure 15.

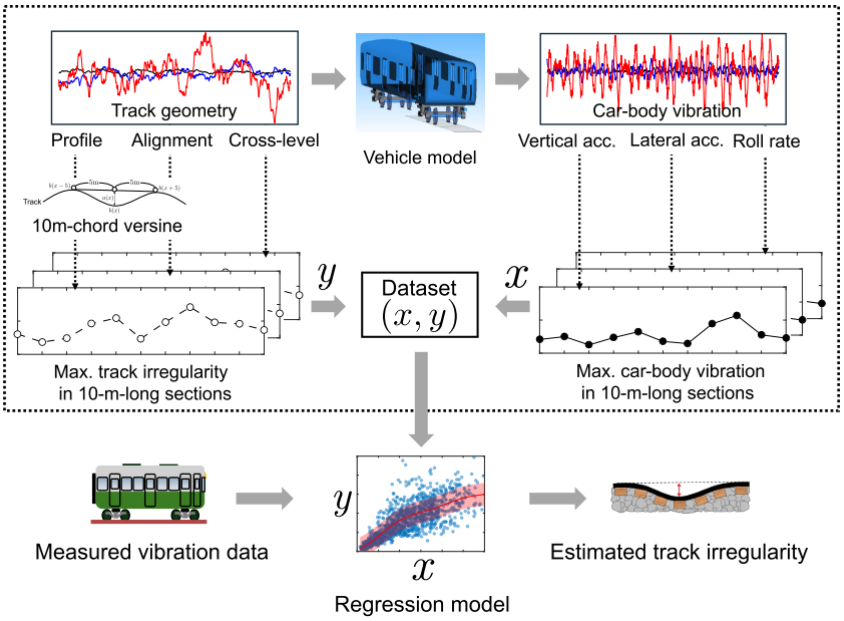


Figure 14 – (TSUNASHIMA; YAGURA, 2024)

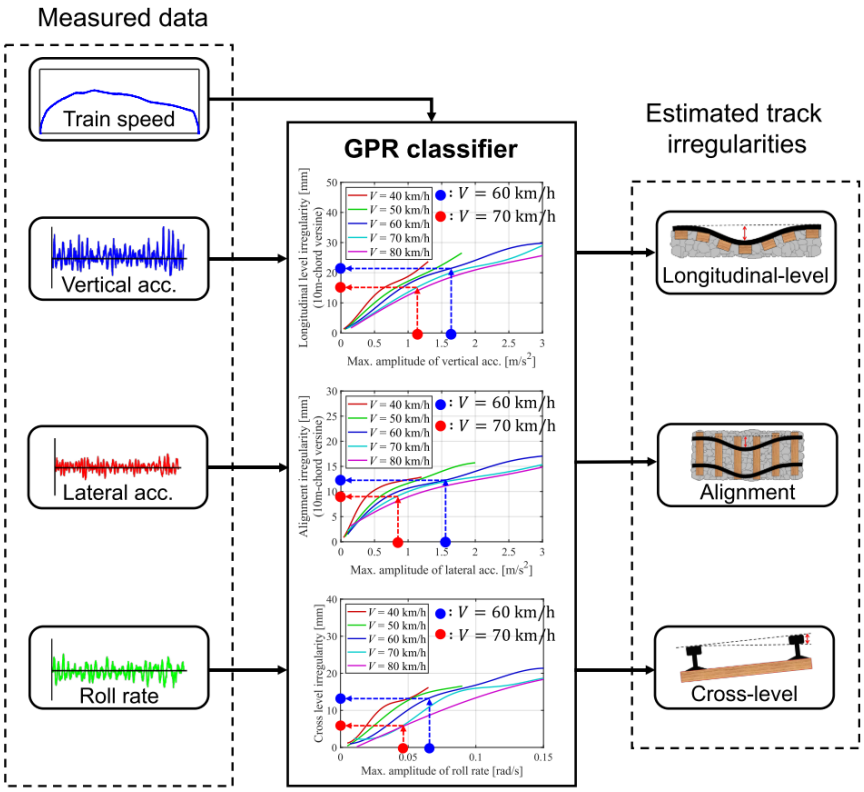


Figure 15 – (TSUNASHIMA; YAGURA, 2024)

The authors then tested their model utilizing real data measured using an onboard sensing device equipped with a triaxial accelerometer, a rate gyro, and a GNSS receiver. To ensure consistency, they applied the same downsample procedure to the real data and averaged the speed in the 10 m section to be used as an input for the regression model. The regression result for one part of the track is shown in Figure 16 and is presented with a 1σ confidence interval.

Tsunashima and Yagura argue that for the majority of the sections, the GPR predicts the correct value within the 1σ confidence interval. However, for some of the sections, the predicted value significantly deviated from the actual measurement. They argue that there is a factor other than the track irregularity that influences the dynamics of the system and superimposes on the carbody's vibration. This difference might also occur because of the low complexity model used that might not have been able to learn the correlations between the variables very well.

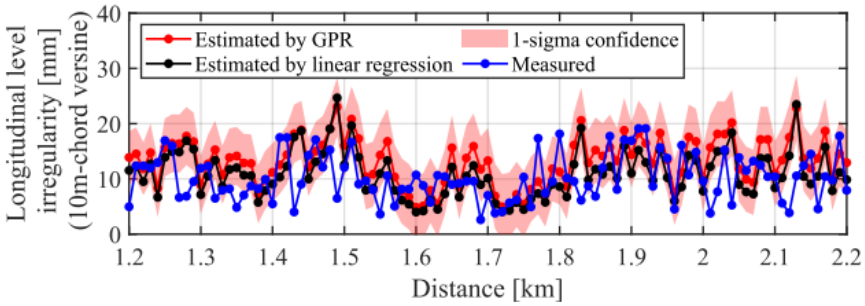


Figure 16 – (TSUNASHIMA; YAGURA, 2024)

In (ROSA et al., 2021), the authors try to develop a threshold to detect not safe railway track irregularities. In the paper, the authors propose a machine learning-based classification model that divides the data into two classes based on the standard deviation of the lateral and roll bogie frame accelerations. Class 1 corresponds to normal conditions, i.e., track irregularities below a defined threshold that do not require maintenance, while Class 2 corresponds to sections with irregularities exceeding that threshold, thus requiring maintenance intervention.

The authors use a dataset composed of real measurements collected onboard the high-speed TGC, operating at 300 km/h, that was also equipped with accelerometers located on the carbody, the bogie frames and the wheelsets, and a set of simulated data generated using a validated multibody dynamics model. From real data, the athor applies a pass-band filter in the range of 3 to 27 Hz and then computed the standard deviation of the signals over 100-meter-long track length. The simulation data was obtained considering a straight track, with a vehicle with speed of 300 km/h and for three different cases of track irregularities: considering only the lateral irregularity, considering only the cross level irregularity, and considering both at the same time. The authors didn't consider vertical irregularities in their simulation. For each case, they ran the simulation 10 times. The standard deviation was computed similarly to the real data. Figure 17 shows the whole dataset, where the red lines shown the standard defined limits for the standard deviation.

Using this dataset, the authors then fitted the data three classifiers: a decision tree, a linear Support vector Machine (SVM) and a Gaussian SVM. Results are shown in Table 1. The authors state that

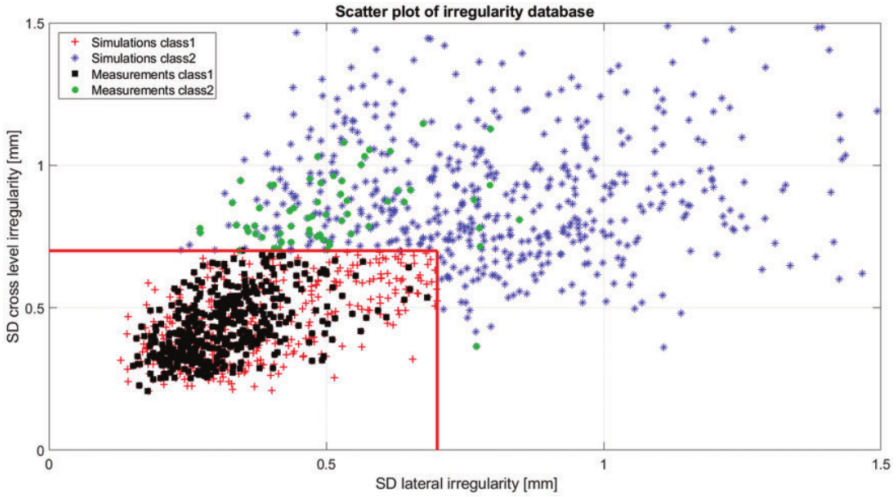


Figure 17 – (ROSA et al., 2021)

	Accuracy (%)	Precision (%)	Recall (%)	F_1 score (%)	Kappa
Decision tree	87.6	49.6	92.1	64.4	0.58
Linear SVM	92.9	70.3	71.4	70.9	0.67
Gaussian SVM	92.9	68.1	77.8	72.6	0.69

SVM: support vector machine.

Table 1 – Summary of classifier performances in the testing phase.

2.14 Identifying Track Defects Using IRVs

3 Methodology

4 Results

5 Conclusion

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Appendix

APPENDIX A – Deriving the Backpropagationg Rule

TODO: Fazer a demonstracao do update dos pesos da Neural network. Usar como base (ROTH, 2016)

Annex

ANNEX A – Morbi ultrices rutrum lorem.

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ANNEX C – Fusce facilisis lacinia dui

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