



ΠΑΝΕΠΙΣΤΗΜΙΟ ΠΕΙΡΑΙΩΣ

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Thesis

**Implementation of the TRACCLUS algorithm
in Neural Networks for vessel trajectory prediction.**

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Abstract

This thesis explores the use of machine learning and clustering algorithms for predicting and improving vessel trajectories. Initially, a machine learning model is trained on vessel trajectory data to predict future vessel locations. Then the trajectories are clustered using a clustering algorithm called TRACCLUS, which groups similar vessel trajectories together based on their location, velocity, and trajectory patterns. The thesis then evaluates the effectiveness of the clustering algorithm by comparing the predicted results of the model before and after the trajectories are clustered. The results show that the use of the TRACCLUS algorithm improves the accuracy of the model, indicating that clustering can help identify patterns and relationships within vessel trajectories that are difficult to identify through machine learning models alone. Overall, this thesis demonstrates the potential of combining machine learning and clustering techniques for improving vessel trajectory predictions and enhancing our understanding of vessel behaviour in marine transportation systems.

*To my professors, supervisor and family
for their unwavering support and help.*

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Chapter 1

Introduction

Maritime transportation systems are necessary for human mobility. An important aspect of maritime transportation systems is the accurate prediction of ship routes. However, accurate ship route prediction poses challenges due to the complex and dynamic changes in marine traffic conditions. Machine learning methods can harness the massive "data explosion" in vessel monitoring to enhance and facilitate the digitization of the shipping industry and address the problem of ship route prediction. This thesis aims to predict the position of ships using machine learning methods and by implementing a trajectory clustering algorithm.

1. Definition of the trajectory prediction problem.

Given a) a trajectory of a moving object: $\{p_0, t_0, p_1, t_0 + Dt_1, \dots, p_i, t_{i-1} + Dt_i\}$, consisting of i transitions of the object, and b) a time interval Dt_{i+1} , the goal is to predict the expected position p_{i+1} of the object at the time $t_{i+1} = t_i + Dt_{i+1}$. Practically, given the "when" component, the goal is to predict the corresponding "where" component, e.g., where the vessel will be in the next few minutes.

Chapter 2

Machine learning and Neural Networks

Machine learning is a branch of artificial intelligence (AI) and computer science that focuses on the use of data and algorithms to imitate the way that humans learn and, through iteration, gradually improve its accuracy. One popular type of machine learning is neural networks. Neural networks are computing systems inspired by the neural networks that constitute biological brains. A Neural Network (NN) is based on a collection of connected units or nodes called artificial neurons, which loosely model the neurons in a biological brain. NNs are able to recognise patterns and data, make predictions, and even generate new data.

1. Machine Learning

Machine learning applies algorithms and statistical models to interpret data and improve performance on a specific task. The main goal of machine learning is the development of algorithms that can make correct predictions on data without being specifically programmed to do so. This can provide deeper insights into problems and a better understanding of the causation and correlation of variables. Fundamentally, machine learning focuses on building models that can generalise and adapt to examples in a dataset, with the goal of making accurate predictions and decisions about new data. The life cycle of machine learning models includes several steps: problem definition, data collection, data preprocessing, model training, model evaluation, model deployment, and model maintenance. In general, the creation and maintenance of a machine learning model is an iterative process with the focus on constant and continuous improvements to achieve optimal performance on the task at hand. There are several different types of machine learning algorithms; the most common types include reinforcement learning, unsupervised learning, and supervised learning. Reinforcement algorithms use a trial-and-error technique and aim to maximise a reward based on their actions. Unsupervised techniques learn from unlabeled data and aim to find patterns and structure in the data; on the other hand, supervised techniques use labelled examples where the input data is associated with the output target data. Machine learning has many practical applications in various domains, including healthcare, finance, marketing, natural language processing, and automotive. Most notably, it has been used for tasks such as image recognition, speech recognition, fraud detection, and driving autonomous cars. In this study, the focus will be on supervised

training and its application to sequential problems. Sequential problems involve using an input sequence to output a prediction. An example of that could be predicting the future values of a time series based on past observations.

2. Neurons | Perceptrons

Neurons, also called perceptrons, are the building blocks of a neural network; in operation, they mimic the neurons of the brain. Within a neural network, neurons are organised into layers. The input layer receives input data, such as an image, number, or text, and passes it to the first hidden layer of neurons. Each subsequent layer processes the output of the previous layer and passes it to the next layer, until the final output layer produces a prediction or classification. Specifically, the neuron is a set of inputs, a set of weights, and an activation function. These inputs can either be raw input features or the output of neurons from an earlier layer. The neuron translates these inputs into a single output, which is then passed through an activation function and picked up as input for another layer of neurons. Each neuron has a weight vector for every input to that neuron. The weights and biases for each neuron are adjusted based on the error between the predicted and actual output during the training stage, such that the final network output is biased toward some preferred value.

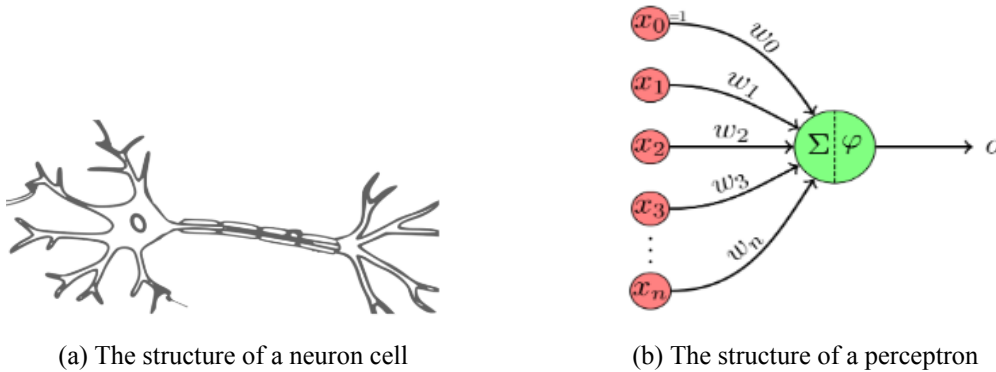


Figure 2.1: The similarities between biological neurons and perceptrons.

3. Activation Functions

The output of each neuron passes through an activation function before continuing to the next layer of neurons. The purpose of an activation function is to introduce nonlinearity into the output of a neuron, allowing the network to model complex relationships between inputs and outputs. Without an activation function, a neural network would simply be a linear regression model. Typically, activation functions are nonlinear and monotonically increasing. Some commonly used activation functions include the sigmoid function, the hyperbolic tangent function, the rectified linear unit (ReLU) function, and its variants such as leaky ReLU and exponential linear unit (ELU). The activation functions can either be differentiable or non differentiable. The choice of activation

function can have a significant impact on the performance of a neural network, and appropriate consideration is given.

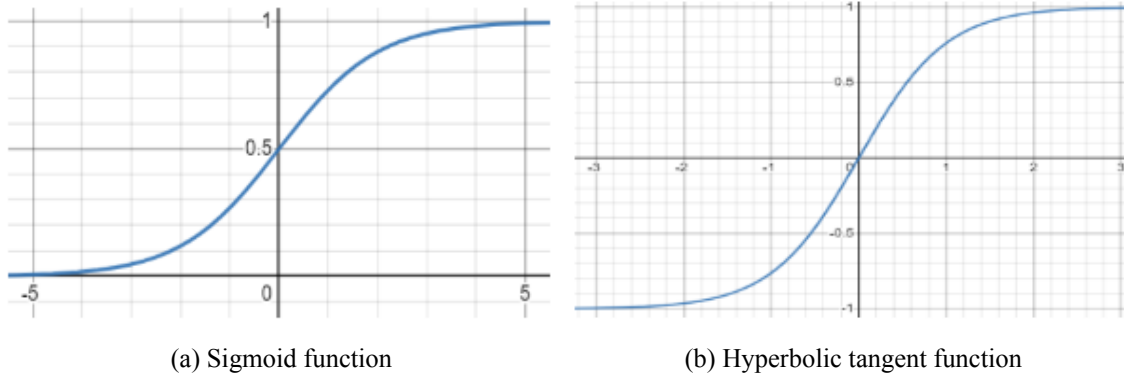


Figure 2.2: (a) the sigmoid function and (b) the hyperbolic function \tanh both examples of differentiable, monotonically increasing functions.

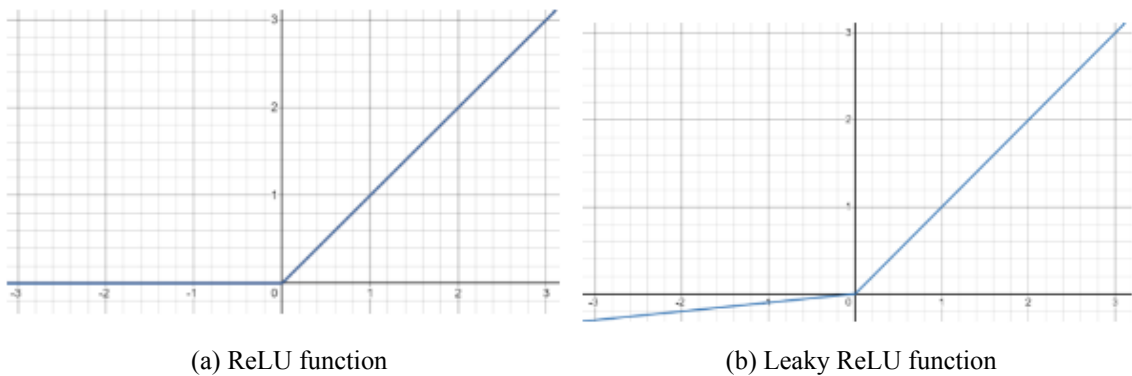


Figure 2.3: (a) the rectified linear unit function and (b) the leaky rectified linear unit function, both examples of non-differentiable, monotonically increasing functions. Non-differentiable functions can create problems with learning, as numerical gradients calculated near a non-differentiable point can be incorrect.

Supervised problems are categorised as classification or regression problems. Activation functions that are commonly used for classification problems belong to the sigmoid family. A sigmoid function is a bounded, differentiable, real function that is defined for all real input values and has a non-negative derivative at each point and exactly one inflection point. Common activation functions in this family are the sigmoid, hyperbolic tangent, and softmax functions.

For regression problems, the goal is to predict a continuous numerical output value. Typically, activation functions for regression problems have piecewise linearity, which further helps calculate a continuous numerical output. Common activation functions for regression problems are the linear activation function, ReLU, Leaky ReLU, and Softplus. Note that the Tanh function is nonlinear but is symmetric around 0 and can handle negative values, making it useful for regression problems.

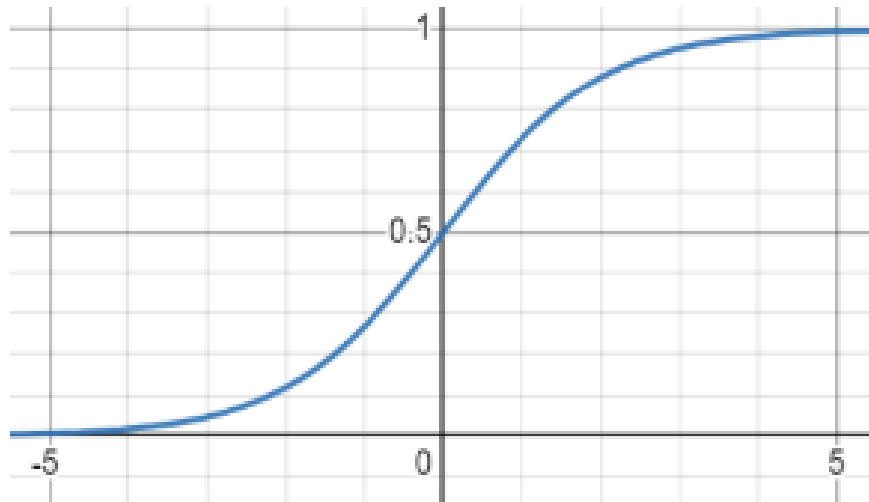


Figure 2.4: The sigmoid function compresses the output into the range $[0, 1]$ most commonly used for binary classification, where the output can be interpreted as the probability of belonging to the positive class. This function has a bias towards 0 and 1.

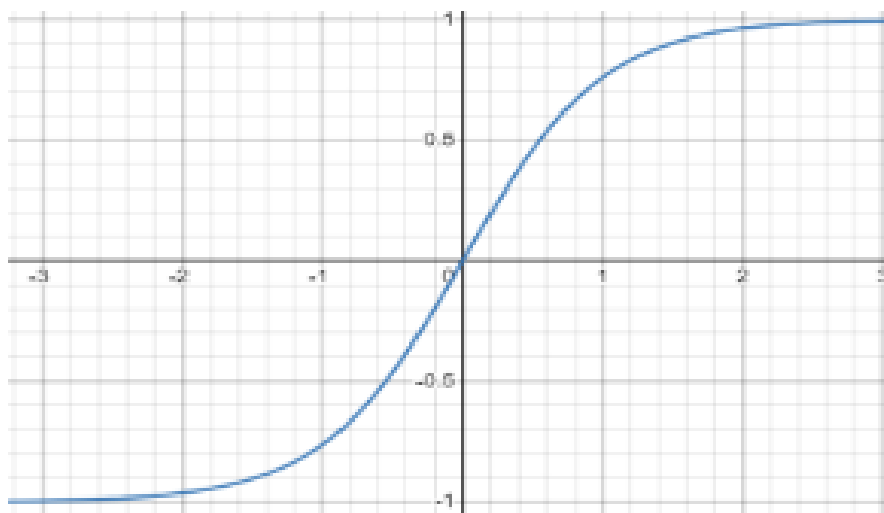


Figure 2.5: The hyperbolic tangent function \tanh compresses the output into the range $[-1, 1]$ most commonly used for classification of zero-centred data or data that also contains negative values. This function has a bias towards -1 and 1.

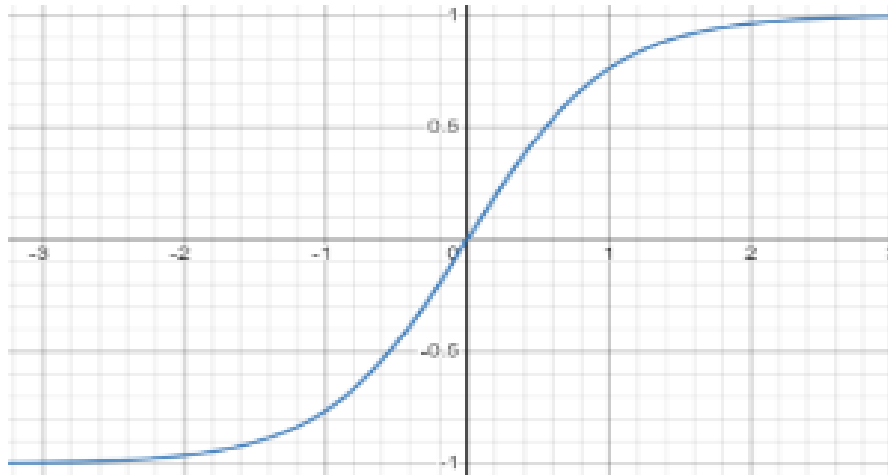


Figure 2.6: The softmax function takes as input a vector of real-valued scores, which can be seen as the evidence for each possible class, and outputs a probability distribution over the classes that sums to 1. The output of the softmax function can be interpreted as the model's confidence in the prediction for each class.

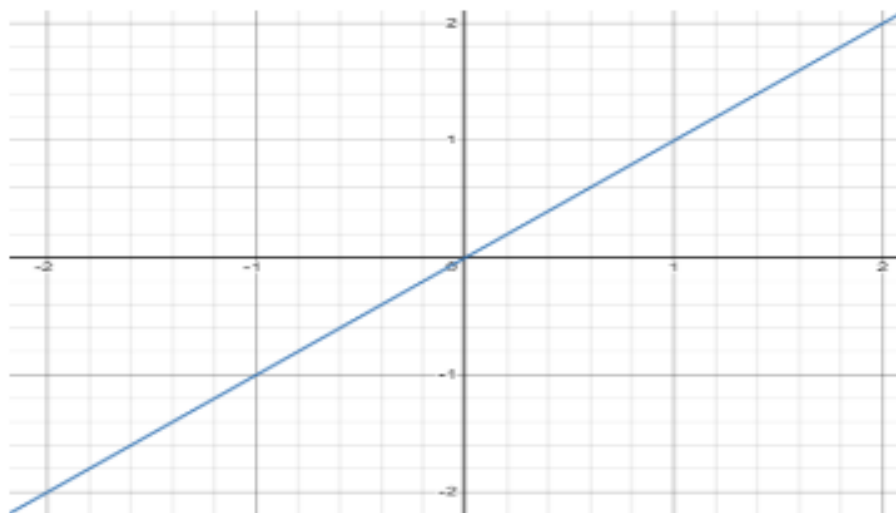


Figure 2.7: The output of the linear function is the input value multiplied by a constant factor and possibly shifted by another constant factor (bias), without any non-linear transformation. $output = (input \times weight) + bias$

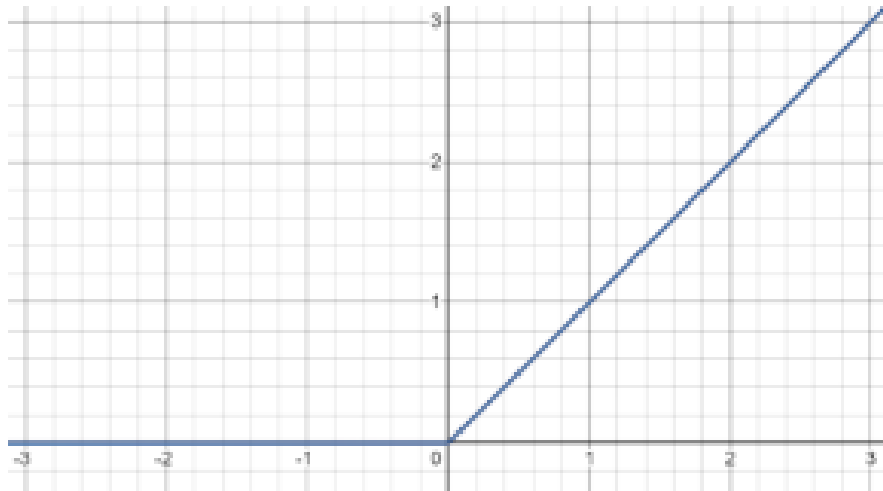


Figure 2.8: The ReLU function returns zero for all negative input values and the input value itself for all non-negative values. This can help introduce non-linearity in the network.

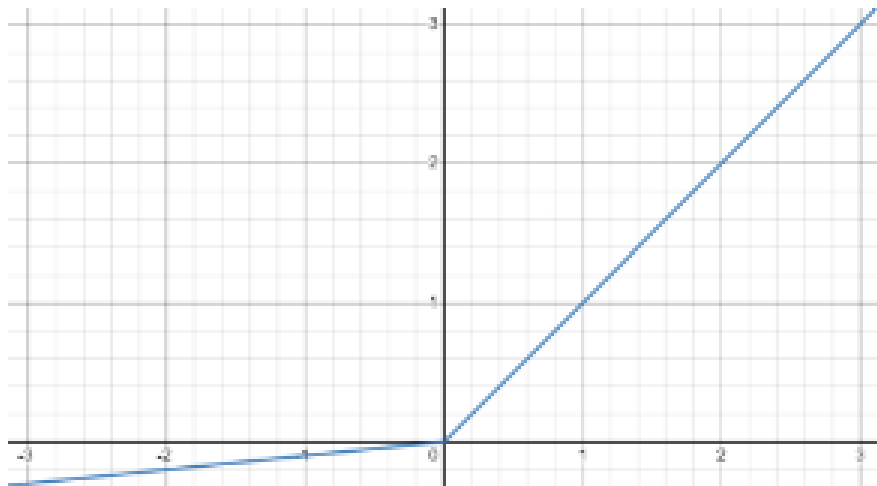


Figure 2.9: The Leaky ReLU is a variant of Relu, with the key difference being that for negative input, it doesn't output 0, but outputs a small constant multiplied by the input value. This prevents neurons from getting stuck with zero output and no gradient being propagated through them during backpropagation, leading to no updates of their weights. (The dying ReLU problem).

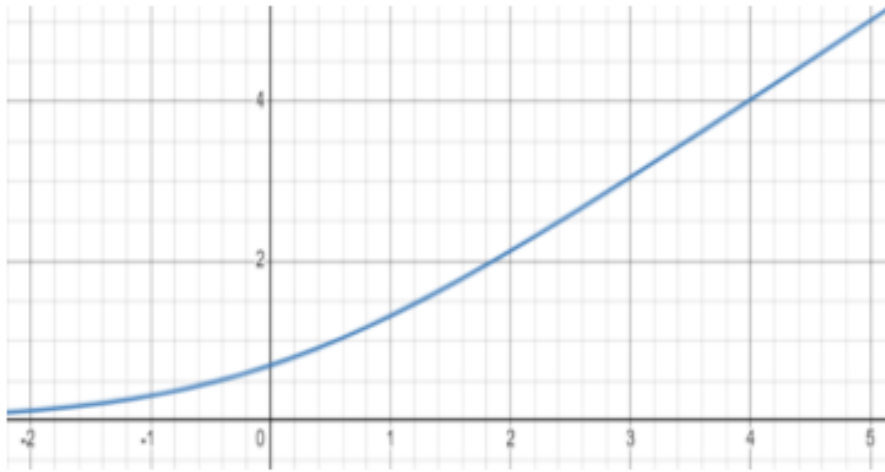


Figure 2.10: The Softplus activation function is similar to the ReLU activation function, but it is a smooth, differentiable function $f(x) = \ln(1 + e^x)$

4. Cost functions

The cost functions are a crucial component in machine learning algorithms. They function as a metric of a model's accuracy and accommodate by guiding towards the best set of parameters that will minimise the error between the actual and predicted outputs during the model's training. Functioning as a representation of the error or cost associated with the prediction, the cost function uses as input the predicted output as well as the actual output and computes a value that the model attempts to minimise. The choice of cost function depends on the specific task and type of model being used. For example, in regression problems where the goal is to predict a continuous value, a common choice of cost function is the mean squared error (MSE). In classification problems where the goal is to predict a categorical label, a common choice of cost function is the cross-entropy loss, which measures the difference between the predicted probability distribution and the true distribution of labels. There exist numerous different cost functions, namely, the mean squared error function (MSE), mean absolute error (MAE), hinge loss, l1 loss, etc. The choice of cost function depends on the specific task and the model being used. For example, in regression problems where the objective is to predict a continuous value, a frequent choice of cost function is the MSE, which measures the average squared difference between the predicted and actual values. Similar to the activation function, the choice of cost function is subject to change, and commonly many different functions are applied, with the most efficient being applied to the final model.

Mean Squared Error	$MSE = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n}$
Root Mean Square Deviation	$RMSD = \sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n}}$
Mean Absolute Error	$MAE = \frac{\sum_{i=1}^n y_i - \hat{y}_i }{n}$
Mean Absolute Percentage Error	$MAPE = \frac{1}{n} \sum_{i=1}^n \left \frac{y_i - \hat{y}_i}{y_i} \right $

Figure 2.11: Commonly used cost functions. Notations: (a) y_i = observed value, (b) \hat{y}_i = estimated value, (c) n = number of data points, (d) i = iterative variable i .

5. Backpropagation

Backpropagation is the algorithm by which the scalar value of the cost function is minimised. It is a method for computing the gradient of the loss function with respect to the weights of the

neural network. Commonly, by using gradient descent or other methods, the network reaches an optimised state. The backpropagation algorithm is based on the chain rule of calculus, which allows the computation of the derivative of a composite function. For example, if the inputs and outputs of the model are a multi-dimensional array of numerical data (tensors) $T_i[m, n]$ and $T_o[j, k]$ each layer of the model can be seen as a function that transforms T_i to T_o . This means that the derivative of the cost function with respect to the weights can be computed by successively applying the chain rule backwards through the layers of the network. Firstly, the input data is passed into the layers of the model, and the output for each layer is calculated with its current weights. Secondly, using the chosen cost function, the error is calculated. Then, the derivative of the loss with respect to the weights of each layer is calculated using the chain rule, starting from the output layer. Lastly, the weights are updated using the computed gradients. This process is repeated iteratively until the network converges on a set of weights that will minimise the loss function.

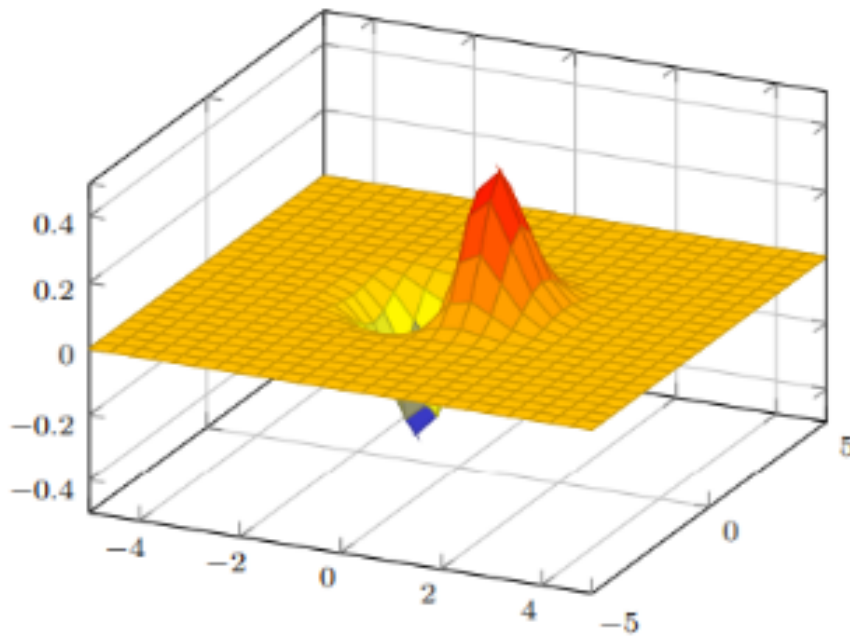


Figure 2.12: A 3d representation of the cost function, the goal of backpropagation is to guide the model to reach the lowest point with regards to cost.

6. Sequential Neural Networks

Sequential neural networks are a type of artificial neural network where the layers of the model are organised in a serial manner. In other words, the output from one layer is fed as input to the next layer, and so on, while the order of the layers stays fixed. As a neural network, it consists of an input layer, hidden layers, and an output layer. The information travels in one direction, from the input layer to the output layer. Each layer processes the information from the previous layer and passes it forward sequentially. As models, they are easy to design and interpret and can model complex nonlinear relationships between the input and output data, making them useful in applications

such as speech and image recognition, natural language processing, predictive modelling, and time series analysis.

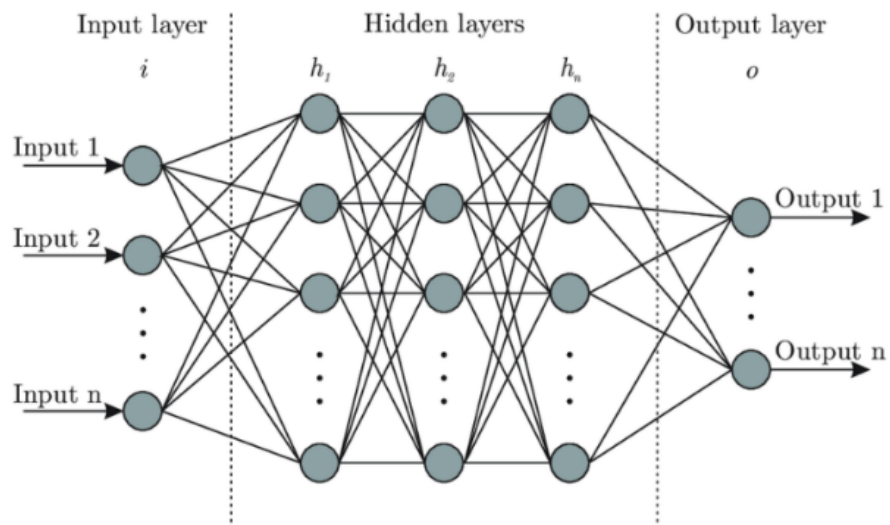


Figure 2.13: A Simple Sequential fully connected Neural Network.
Published in: Python in Plain English, Apr 30, 2020

Chapter 3

Data Analysis and Visualisation of Trajectories

Trajectories are a key concept in machine learning. Understanding the trajectories of objects can help in predicting the behaviour of complex systems and optimising the performance of machine models. Geographical trajectories can inform policy and decision-making in areas such as urban planning, transportation, and emergency response. Mostly, they are influenced by a range of factors, including geography and climate. In order to study geographical trajectories, extremely large datasets need to be analysed (Big Data) and various tools and techniques are applied, namely visualisation tools such as Geographic information system (GIS) and Automatic Identification System (AIS).

1. Big Data

Big Data are extremely large datasets that are too complex or varied to be analysed using traditional data processing tools. They can be generated from various sources, such as social media, online transactions, and sensor networks. The main features when mentioning big data are the 3 Vs (volume, velocity, and variety). Volume refers to the size of the data; velocity is the speed at which these data are generated and need to be processed; and variety refers to the diverse range of data types inside the dataset. Big data has become important in recent years due to the rise of new technologies that allow the creation, manipulation, analysis, and processing of large datasets. The challenge of processing and analysing such datasets is the epicentre of many studies in the field of computer science.

2. Geographic Information System (GIS)

GIS stands for Geographic Information System. It is a powerful computer system used for capturing, storing, analysing, and displaying geographically referenced information. GIS software

allows users to create maps and perform spatial analyses to gain insights into complex phenomena and relationships between different geographic features. GIS data can be acquired from a variety of sources, such as satellite imagery, GPS data, and ground surveys. GIS can help with combining and integrating the data sources in order to create a comprehensive and detailed visualisation of a particular phenomenon in a geographic area. Overall, it is a powerful, versatile tool with a wide range of applications.



Figure 3.1: E. W. Gilbert's version (1958) of John Snow's 1855 map of the Soho cholera outbreak showing the clusters of cholera cases in the London epidemic of 1854 one of the earliest successful uses of geographic information analysis.

3. Automatic Identification System (AIS)

The Automatic Identification System (AIS) is a technology used in the maritime industry that uses transceivers, radio signals, marine radars, and sometimes satellite signatures to track and identify vessels in the surrounding area and share this information with nearby vessels and authorities. The vessels using AIS broadcast real time information such as position, course, speed, and vessel identity, which is collected and sent to a central database to be accessed and used by authorised users. Its main uses are collision prevention, fishing fleet monitoring, accident investigation, and search and rescue missions. Furthermore, it can be used to monitor vessel traffic and improve shipping routes through the use of computer algorithms. Some potential limitations of AIS fall in the fields of data privacy, cyber attacks, signal jamming, and the possibility of data emission errors. However, AIS is an important technology that continues to develop in order to improve safety, efficiency, and sustainability. In conjunction with GIS, it is a powerful tool that can help create

machine learning models for trajectory prediction, autonomous shipping, and dynamic collision avoidance.

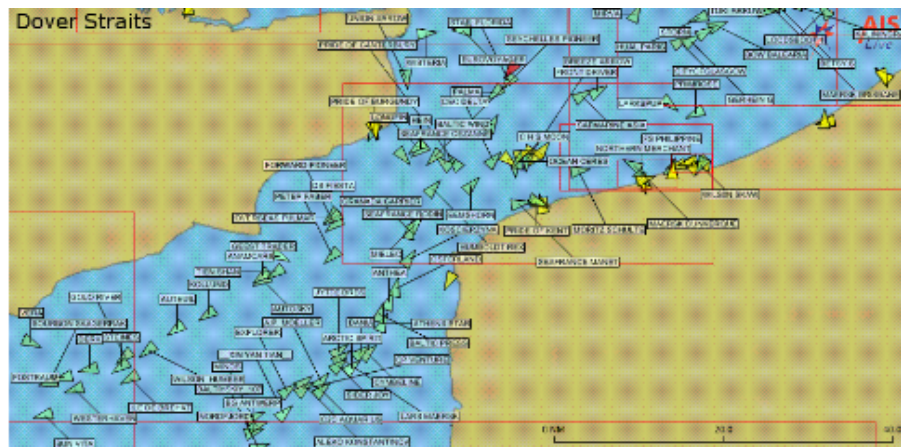


Figure 3.2: A graphical display of AIS data on board a ship.

Chapter 4

Literature Review

The Trajectory Prediction (TP) problem has received a lot of attention in recent years. This general problem can be further classified into two subfamilies: short-term prediction and long-term prediction [1, 2]. The focus of short term prediction models is on predicting the object's next location precisely, whereas long term prediction focuses on predicting possible next locations and routes. The proposed combating methods are mostly Machine Learning (ML) methods that are hybrid in nature, and their components fall into three categories: rule-based prediction approaches, clustering-based prediction techniques, and predictive analytics methods. [3, 1]

1. Combating methods for the TP problem

There are several methods for combating the trajectory prediction problem. In this section, we will analyse each approach and provide their strengths and weaknesses.

1..1 Neural Networks (NNs)

A plethora of research has been done, expanding on the methods mentioned in Chapter 2. As proposed in [4, 5, 6] rigorous experiments have been conducted, applying numerous different NN models. It is derived that using NN models provides us with high accuracy, especially when dealing with complex patterns and large datasets, due to the non-linear relationship modelled between features in NN models. Additionally, NNs tend to be robust and able to handle noisy and incomplete data, making them ideal for handling data without the need for manual feature engineering after they learn the relevant features from raw sensor data. Neural networks can be categorised as static or dynamic. Static neural networks have a fixed architecture, and the weights and biases of the network are pre-determined before the network is used for inference. In contrast, dynamic neural networks have an adaptive architecture where the network can change during inference based on the input data. In tasks with fixed input sizes, such as the one we are studying, static neural networks are commonly preferred. Unless it is specified beforehand, from this point on, when a neural network is referred to, it is implied as a static NN. Below, we will expand on the tools used to

create NNs for the Trajectory Prediction problem.

1.2 Rule-Based Methods

Using rule-based predictions is of great help in TP problems, especially when the nature of the problem requires limitations such as the road network and aircrafts moving in airway space. Sadly, aquatic vessels sail with a 2D flexibility that is derived from the non-fixed and sparser seaways. [3] Although rules are crucial for predictions, their application to aquatic vessels is limited due to the nature of maritime travel.

1.3 Clustering-Based Methods

Further facilitation of a NN to increase accuracy usually comes in the form of clustering. Especially in aquatic vessels where rule based methods are limited; clustering based methods have a greater role in the improvement of the model. Clustering based methods sacrifice time at the initial stages of building the NN models in order to properly feed the model with well clustered data that will raise the model's accuracy. Notable methods used for clustering are Traj-clusiVAT [1] where the technique was created and used to handle big data to create a scalable trajectory classification technique used for both short-term and long-term predictions. DBSCAN is also a commonly used technique that can be implemented on all data points to create multiple path corridors derived from representative trajectories. As made clear in [4] the knowledge of both trajectories and common sub-trajectories is used to extract crucial data that can further facilitate the NN models. Furthermore, a clustering method like TRACCLUS [7] can create simplified representative trajectories from all the data points and find common sub-trajectories based on trajectory line density. In this study, the methodology will delve deeper into the TRACCLUS method, which will be the primary area of focus.

1.4 Predictive analytic methods

Predictive analytics can be used to analyse big data streams and predict, based on historical data, the future behaviours of objects. In [8] the importance of feature selection and data sampling using decision Trees random forest and support vector machines is highlighted in order to improve the performance of models. In [3], the predictive analytics framework based on LSTM NNs can be used in a variety of applications, such as maritime traffic management, ship routing, and marine safety. The authors highlight its ability to predict future locations of vessels based on learned patterns and compare it with other machine learning models to demonstrate its superiority in terms of efficiency and accuracy. Predictive analytics are also used in [4] in the form of tools such as heat maps and trajectory analysis, to make predictions from data derived from big data technologies, such as Hadoop and Spark, using machine learning algorithms, like random forest and gradient boosting to predict the likelihood of illegal fishing. The i4sea platform is a practical application of predictive analytics that can be also applied in many marine conservation and management domains.

1.5 Markov Models

Markov Models(MMs) are a type of probabilistic model that can be used for sequence prediction tasks such as speech recognition and natural language processing [9] . Existing methods for the TP problem are based mostly on data-driven methodologies, such as Hidden Markov Chains and Neural Networks (NN) [3] . An example of Markov models can be seen in [1] where a combination of MMs and NN models were used to predict the trajectories of objects such as vehicles, pedestrians, and animals. To address the limitations of existing approaches, they used a hierarchical approach that combines MMs and NNs. The MMs capture short-term dependencies in the trajectory data, while the NNs capture long-term dependencies, thus providing more accurate predictions overall. A similar approach can be seen in [10] where the study proposes a hybrid model that combines a feedforward neural network with a Markov model. The neural network is used to capture long-term dependencies in the trajectory data, while the Markov model is used to capture short-term dependencies.

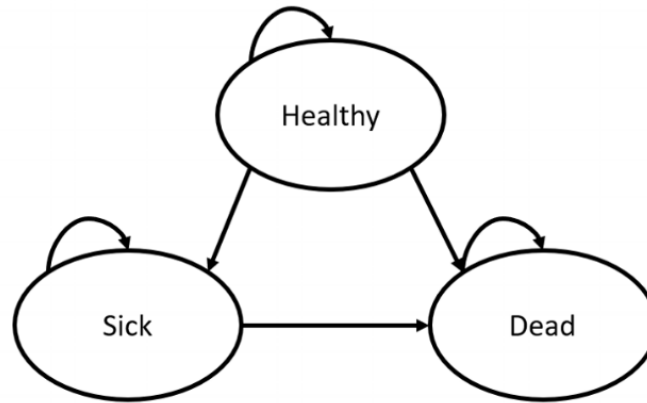


Figure 4.1: A three state Markov Model.

Published in: Generating Survival Curves from Study Data: An Application for Markov Models (Part 2 of 2), Mark Bounthavong March 15, 2018.

2. Drawbacks

Although the methods referenced in Chapter 4.1. are used due to their competence and efficiency in solving the TP problem, this section will focus on and analyse their general drawbacks.

2.1 Drawbacks of Machine Learning models

Under certain circumstances, ML models are prone to underperform when the quality or quantity of the data is subpar. This often happens when the data used is noisy or incomplete. Extensive care must be taken by the researcher to avoid using data that is not fit for a ML model. In some cases, the

models created can be difficult to interpret, making it challenging for the researcher to understand why the model is making certain predictions, which is especially problematic in domains where the reasoning behind the prediction needs to be understood. In regards to the training process, special attention is given to avoiding overfitting, which can lead to poor performance on test data and an inability to generalise on new data. During the model-designing process, the training data is extensively checked to avoid bias and address fairness concerns to ensure that the resulting model is developed in a way that is fair and unbiased. Lastly, the algorithm selection process can be challenging, and selecting the appropriate one can be difficult since different algorithms have different strengths and weaknesses, and a poor choice can lead to poor results.

2..2 Drawbacks of Clustering Techniques

Clustering-based techniques are often based on distance measures and are sensitive to noise and outliers, especially if those are not handled correctly. Additionally, their simplistic nature makes them unable to capture complex relationships between variables, which can cause underfitting. They usually require a posteriori knowledge of the optimal number of clusters [3], which may not be known a priori, and an incorrect choice of cluster number can lead to inaccurate predictions. In regards to clusters, points in the same cluster are treated as similar between them and dissimilar with points in other clusters, which, in practice, may not be the case since clusters can be overlapping or have non-uniform densities. Lastly, they are not well suited for time-series problems due to their lack of understanding of temporal dependencies between data points, leading to inaccurate predictions when the nature of the data contains complex patterns or trends.

2..3 Drawbacks of Predictive analytics methods

Predictive analytics methods, such as Markov Models and hidden Markov Models, have proven to be very useful in making predictions, but their predictive ability is confined to the data that is used to train the model, giving them a limited scope [10]. If the data is not representative of the general population, the predictions will not be accurate. Furthermore, it is important to note that regression models can only identify correlations between variables, not causation. Thus, predictions by the model should be interpreted with caution, as there may be underlying variables that are not captured in the model. Finally, variables with nonlinear relationships are not properly understood by models using predictive analytics in view of the fact that they assume linearity between input variables.

2..4 Drawbacks of Markov Models

Specifically, Markov models assume that the probability of an outcome depends on the previous state, disregarding more complex relationships of higher order between variables. This in turn shows the model's dependency on the initial conditions; if the initial conditions are not accurately known, the predictions are unreliable. Even with those factors accounted for, Markov models do not have the ability to update the probability distributions of their states over time, and they assume that the future is independent of the past, being unable to take into account the history

of the process beyond its current state [3] . Lastly, their dependability on large sample sizes to estimate the transition possibilities between states makes them unreliable for smaller sample sizes.

2..5 Drawbacks of rule-based algorithms

In general, applying pre-defined rules to the data can make the algorithm inflexible and unable to adapt to changes in the data or new scenarios. Also, the complexity of the rules can make it challenging to interpret the predictions or identify the rules that contribute the most to the predictions. Lastly, applying rule based algorithms implies that the rules applied capture all the relevant features of the data, which can be difficult to estimate in complex systems and can create an inability to handle noise and outliers, which sequentially impacts the performance of the model.

Chapter 5

Methodology

In this study, we developed a method to predict the future trajectories of maritime vessels by applying a clustering algorithm that clusters similar trajectories together and then training a feed forward neural network that predicts the future positions of vessels based on the cluster they belong to. To evaluate the results, we compare the method's accuracy with the results of a sequential neural network without clustered data. The following sections describe in detail the data, tools, and techniques used in this study to carry out trajectory prediction with the use of NNs and trajectory clustering with the TRACCLUS algorithm [7].

1. The data

The data used is from passenger ships for the month of January 2018. The focus will be on the Aegean Sea. Identifying the longitude and latitude values that will be the boundaries of the region in question will help clean the data from outliers. The boundaries of the Aegean Sea are not fixed and can vary depending on the source of information. Arbitrarily, the rectangle created from the coordinates 35.660669° N, 39.517331° N, 23.088642° E and 26.896934° E encompasses a large part of the Aegean Sea and fragments of the surrounding landmass.

2. About Data Preparation

Data preparation/Wrangling refers to the process of preparing data for training and testing machine learning models. This includes tasks such as data cleaning, data transformation, data encoding, and data splitting. The goal of data preparation for machine learning is to ensure that the data used to train the machine learning model is of high quality and can be effectively used to learn patterns and relationships in the data. Data preparation is considered one of the most time-consuming and crucial steps in the life cycle of a ML project. Given a raw dataset, data preparation involves the process of removing errors, checking for inconsistencies, and in general, ensuring reliability, accuracy, and consistency across the dataset.

Table 5.1: Sample Preprocessed Data [10.283.171 rows x 8 columns].

mmsi	timestamp	lon	lat	shiptype	speed	course	heading
355931000	2018-10-02 20:11:12	23.870230	37.402481	60	174	341	341.0
237233600	2018-10-02 20:11:14	25.740101	35.007332	65	0	359	511.0
237294700	2018-10-02 20:11:16	23.542440	37.959049	60	71	86	511.0
271041325	2018-10-02 20:11:16	27.429489	37.034210	60	0	0	511.0
271002606	2018-10-02 20:11:16	27.954029	40.355400	60	0	0	511.0
...
237641000	2018-10-02 20:10:56	23.869181	37.349380	69	200	157	151.0
249727000	2018-10-02 20:11:01	24.457350	38.598270	60	141	316	316.0
237032000	2018-10-02 20:11:07	24.736830	35.937832	60	206	327	328.0
271044139	2018-10-02 20:11:07	28.730591	40.890369	60	108	323	511.0
239575000	2018-10-02 20:11:07	23.834829	37.381168	60	188	158	158.0

2.1 Data preparation

Since a regional window was already chosen, the first step will be to delete all rows from the dataset that are beyond the window that is allowed. Regarding the homogeneity and standardisation of the data, care is given to every column, and duplicate rows are deleted. e.g., timestamps are converted to unix integers with a datetime pandas conversion, and longitude and latitude degrees are turned to WGS84 decimals. Columns that are considered unnecessary or do not inspire confidence will be deleted, e.g., the speed column. Lastly, columns that will be helpful later on are added, e.g., the column dt, which denotes how much time has passed from one signal to the next, and the new speed column.

2.2 Further Data Preparation

After completing the basic data wrangling mentioned above, further preparation is applied to the data. The trajectories of the ships that are denoted by their MMSI identification are split based on logical assumptions. A trajectory cannot be less than 10 timesteps or more than 1.000 timesteps, and if there is a gap between signals of more than 30 minutes, the trajectory is split at that point. Furthermore, a trajectory cannot last more than 24 hours. Regarding the vessels' speed, if the speed is less than 0.1 nautical knots, it is considered stopped; the trajectory is then split and the row is deleted. Finally, if the speed is greater than 25.7 nautical knots, it is considered unrealistic, and the trajectory is split. This process is iterative and continues until no further changes are made by the program. For the final step, basic data analysis is applied, the dataset is shuffled to avoid overfitting when training, and it is split into three parts for training, validation, and testing. Overall, data cleaning is a critical step in the data analysis process that ensures that the data is reliable, accurate, and consistent and can be used for further analysis or modelling. Data cleaning requires careful attention to detail and a solid understanding of the data and the problem being

solved.

2.3 Converting timeseries to a supervised learning problem

Given a timeseries with 3 variables X, Y, Dt where X is the longitude, Y is the latitude, and Dt is the time difference from one timestep to the next, the goal is to create $n \times 3$ new columns, where n is the number of lagged timesteps we want to create. Every new column will be the same as its predecessor but shifted by one step. For the purpose of this research, a step of $n = 10$ is used, resulting in 156 columns. At this point, the dataset is checked to avoid rows that contain trajectory identities that do not match. After further cleaning and removal of redundant columns, the dataset left contains, in total, 66 columns. This technique is commonly used for machine learning; converting the dataset to a tabular form helps create a table where every row contains information about the object for the last n observations. The rows of the dataset that contain missing values are removed, and the resulting table is split into two tables, one of observations $(t - 10) \dots (t - 9)$ and one of observations (t) . The first will be used as the input of our algorithm, while the latter will be the goal output of the supervised problem. This tabular conversion is a powerful tool that helps make accurate predictions based on past observations. Lastly, the two datasets created are split into training, validation, and testing sets to further accommodate solving the supervised problem. The training set will be the set on which the model will train its parameters, while the validation dataset will be the control set that judges accuracy and helps avoid overfitting. Lastly, the testing set will be the dataset that will judge the general accuracy of the model with data it has not seen yet. Of the original set, 55% will be used as the training set, 15% will be used as the validation set, and 30% will be used as the testing dataset.

3. The Neural Network model architecture

When attempting to create a neural network model, various parameters have to be considered. A dense sequential neural network was chosen due to its simplicity, training speed, and flexibility. The architecture of the model consists of an input layer with 42 variables, 4 dense hidden layers with populations of 32, 16, 8, and 4 neurons, respectively, and an output of 2. Various layer compositions were tried. This decreasing layer approach was chosen to extract increasingly abstract features from the input data, making it effective in capturing important feature points while minimising the risk of overfitting. The data were scaled before passing through the model, depending on the activation function used each time. The best results were given when using a standard scaling of range $[0, 1]$ and the ReLU activation function for every layer. Regarding the hyperparameters of the model, the chosen cost function was the mean absolute error (MAE) and the mean squared error (MSE) while the optimising method used was an extended version of stochastic gradient descent called Adam optimiser. Although the Adam optimizer requires more computational power, it has some benefits, making it a better choice for the problem at hand. Some benefits of the Adam optimizer against stochastic gradient descent are its ability to use adaptive learning rates for each weight and its ability to use both gradient and momentum to update the weight parameters. Finally, regarding the iterations of the training process, two methods were used. A check mechanism that compares the accuracy of the validation data of the current epoch with the validation accuracy of

mmsi	trl_val2_test3	id	WGS84lon	WGS84lat	t	lon	lat	dist_m	dlon	dlat	dt	speed
237018400	1	1	23.530130	39.166431	1527491036	200205.617017	4.340983e+06	1086.690420	869.729229	651.511426	171.0	6.354915
237018400	1	1	23.538771	39.171829	1527491194	200975.271999	4.341554e+06	958.158259	769.654983	570.699970	158.0	6.064293
237018400	1	1	23.549900	39.178848	1527491404	201966.648647	4.342296e+06	1238.622488	991.376647	742.534856	210.0	5.898202
237018400	1	1	23.558029	39.183849	1527491555	202690.132658	4.342825e+06	895.938895	723.484012	528.467018	151.0	5.933370
237018400	1	1	23.569630	39.191471	1527491774	203724.494176	4.343633e+06	1312.623793	1034.361518	808.132089	219.0	5.993716
...
240080500	3	53715	23.543800	37.959721	1524390974	196343.777405	4.206983e+06	403.029610	-400.377580	-46.159074	123.0	3.276663
240080500	3	53715	23.538919	37.959450	1524391102	195913.693696	4.206969e+06	430.315890	-430.083709	-14.133955	128.0	3.361843
240080500	3	53715	23.534700	37.960499	1524391227	195547.244059	4.207099e+06	388.906798	-366.449637	130.242700	125.0	3.111254
240080500	3	53715	23.531450	37.964001	1524391362	195276.115323	4.207499e+06	482.708402	-271.128736	399.370267	135.0	3.575618
240080500	3	53715	23.530300	37.965599	1524391501	195181.669898	4.207680e+06	204.291116	-94.445425	181.148894	139.0	1.469720

Table 5.2: The data after processing

Table 5.3: Example mock Timeseries problem.

Longitude X	Latitude Y	Time Dt
1	1	1
2	2	2
3	3	3
4	4	4
5	5	5
6	6	6
7	7	7
8	8	8
9	9	9

Table 5.4: Example mock Timeseries problem converted to supervised problem of lag timesteps 2.

Longitude X_{-1}	Latitude Y_{-1}	Time Dt_{-1}	Longitude X	Latitude Y	Time Dt
1	1	1	2	2	2
2	2	2	3	3	3
3	3	3	4	4	4
4	4	4	5	5	5
5	5	5	6	6	6
6	6	6	7	7	7
7	7	7	8	8	8
8	8	8	9	9	9
9	9	9	Nan	Nan	Nan

Table 5.5: The input of the algorithm.

dlon(t-10)	dlat(t-10)	speed(t-10)	dt(t-9)	dlon(t-9)	...	dt(t)
678.048594	-265.691638	4.887556	141.0	616.915065	...	131.0
616.915065	-296.483109	4.854331	220.0	616.915065	...	131.0
955.288911	-440.407878	4.781455	131.0	577.215446	...	60.0
577.215446	-233.752623	4.753819	140.0	615.886767	...	220.0
615.886767	-211.968419	4.652447	149.0	606.261439	...	180.0
...

Table 5.6: The goal output of the algorithm.

dlon(t)	dlat(t)
676.550407	-198.792543
633.754767	-178.405028
592.817516	-164.923137
582.374405	-194.422268
616.910006	-206.865550
...	...
27.187918	-996.591755
-62.082231	-992.105461
-357.689199	-1269.006625
-473.783384	-622.380551
-573.308693	-307.355356

the previous epoch; if the new weights are more accurate, they are saved; and a patience parameter of size 10 that checks if any meaningful improvements have been made; if for 10 consecutive epochs no meaningful improvements are made, the iteration stops. The model showed best results in the range of 21 to 35 iterations.

4. Clustering trajectories

In order to understand the process of trajectory clustering, an understanding of general clustering is needed first. There are three main factors to take into account. Firstly, the distance metric; when clustering data points, a metric is needed to judge if points should be clustered together. Secondly, the clustering algorithm; in this study, an algorithm based on density, Traclus, was chosen [7]. Lastly, the number of clusters that best suit the problem at hand.

5. Representative trajectories

Regarding trajectories, the first action needed for computational speed is to create representative trajectories. In this Chapter, the dataset was created, and every trajectory was given a characteristic identity. Given the spatiotemporal points of a trajectory, a simplified representative trajectory can be extracted without sacrificing much in terms of accuracy. The goal is to partition every trajectory of n points into its characteristic points to create a representative trajectory with fewer points. This process requires the use of the minimum description length principle (MDL). The program traverses the trajectories sequentially, and at every point it computes the difference between the real trajectory and a linear trajectory from the origin point to where it is currently located. If the cost of partitioning is greater than not partitioning, then the point prior to the one the program is currently

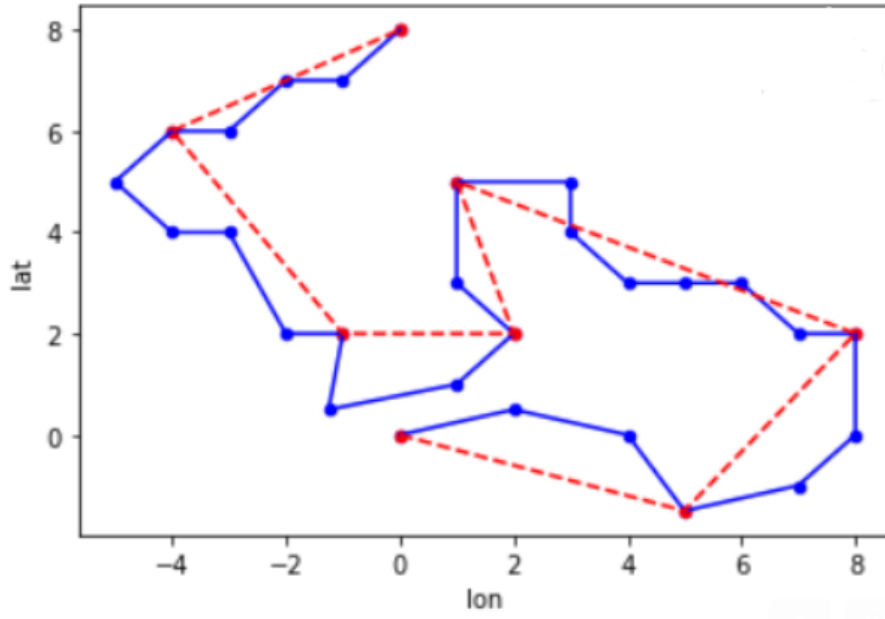


Figure 5.1: blue: An example trajectory of n points.
red: the representative trajectory made from j characteristic points

checking is considered a characteristic point. The number of traversed points is set to 0, and the new characteristic point is now considered the origin. The program continues until there are no more trajectories to check and creates a new dataset of characteristic trajectories. To accomplish

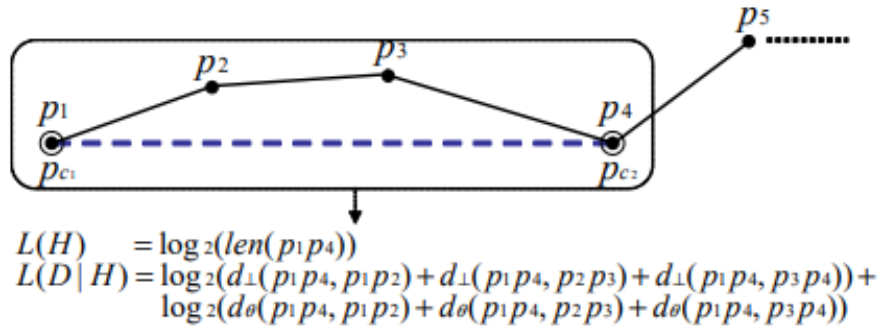


Figure 5.2:

Formula of the MDL cost. $L(H)$ is the hypothesized partition. $L(D|H)$ is the sum of the difference between a trajectory and a set of its trajectory partitions p_1, p_2, p_3, p_4 . The best hypothesis minimises the sum $L(H)(D|H)$

d_{\parallel} = parallel distance, d_{\perp} = perpendicular distance, d_{θ} = angular distance

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the goal mentioned, the creation of a distance function is needed. The distance function was made up of three components. the perpendicular distance, the parallel distance, and the angular distance.

The perpendicular distance is provided by the Lehmer mean; the parallel distance is the minimum distance between the origin of the line and the first projection of the line segment on it, and the second projection up to the end of the line. Lastly, the angular distance is defined as the sine of the angle between the real line and the representative line times the length of the real line. The sum of the three distances is considered the total distance between two lines .

$$dist(L_i, L_j) = w_1 \times d_{||}(L_i, L_j) + w_2 \times d_{\perp}(L_i, L_j) + w_3 \times d_{\theta}(L_i, L_j) \quad (5.1)$$

In this study, when applying the (5.1) formula, the weights w_1, w_2, w_3 are considered equal to 1.

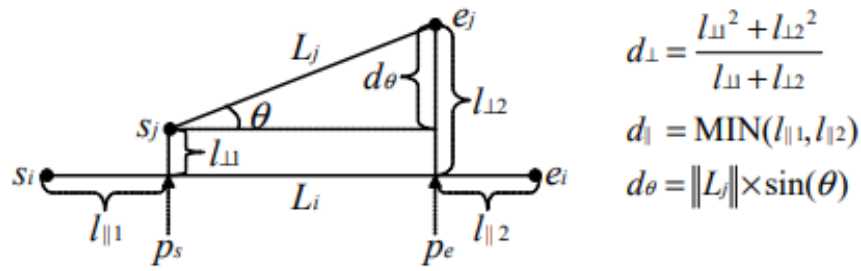


Figure 5.3:

Example of the three distance metrics. If $\theta > 90$ we consider $\sin(\theta) = 1$.

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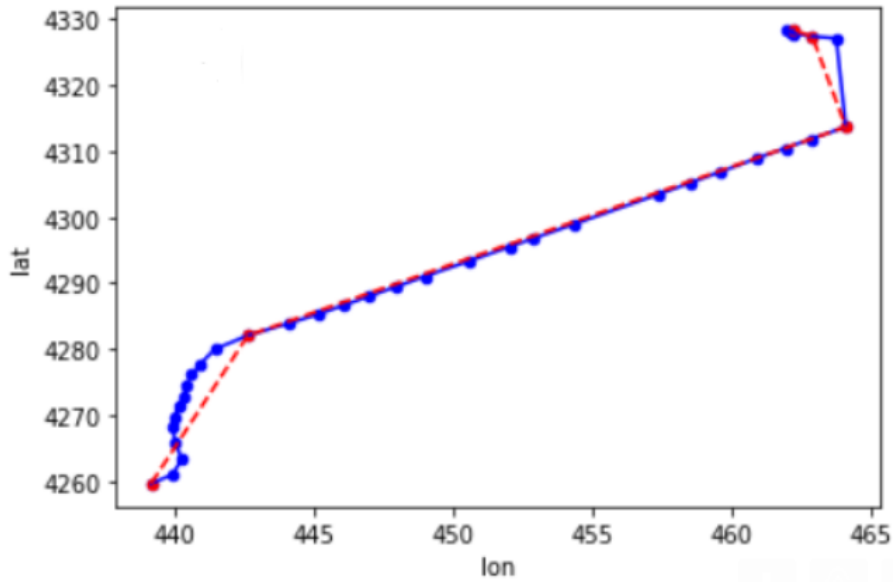


Figure 5.4:

Result of a real trajectory partitioning.

5.1 clusters of representative trajectories

After performing the actions mentioned above, the resulting product is a dataset containing each characteristic line. In order to continue and perform the clustering on the trajectories, a new dataset is created containing the distances used in Figure 5.3 between all characteristic lines. This dataset will be crucial for applying the altered DBSCAN algorithm to the line segments and will help to calculate the heuristic parameters of ϵ and MinLns. The ϵ parameter is the distance threshold that is used to define a radius around each line in the dataset; in this case, the radius results in transformed ellipses. Lastly, MinLns is the parameter that specifies the minimum number of lines that must be within the epsilon radius of a core line in order for that line to be considered a part of a cluster.

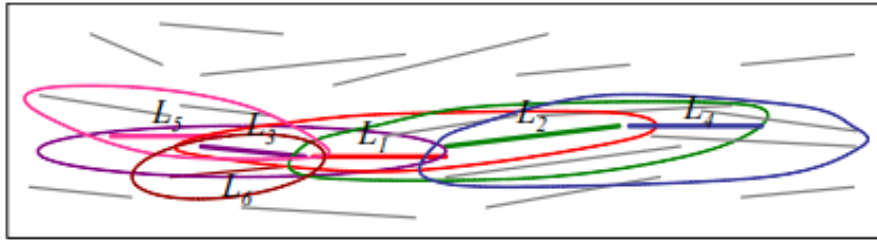


Figure 5.5: Example of the DBSCAN algorithm on line segments.

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5.2 calculating the hyperparameters

As mentioned, the ϵ parameter is the distance threshold that is used to define the radius around each line. In order to find the optimal ϵ value, the entropy formula is used. Entropy is a measure of the disorder or randomness in a system, and it is used to quantify the amount of uncertainty or unpredictability in a set of data. The goal is to choose an ϵ value that minimises the entropy of the system. To achieve that, the entropy of the dataset is calculated for a range of ϵ values, and a value that results in the minimum entropy is used. It is important to notice that the ϵ value is not the one that gives the least entropy, but rather a value around the region of least entropy that gives the most meaningful clusters. After calculating the optimal ϵ the average line neighbours of that ϵ value are calculated, and the MinLns value is chosen. Since the clusters that are to be created have to be meaningful, it is a logical assumption that $\text{MinLns} > \text{AvgNgb}$. In order for the MinLns chosen to be impactful, just like the ϵ value, it is chosen based on the clusters it creates. The clusters created are judged on their population and their cardinality. A healthy cluster must contain a healthy population of trajectories of different identifications; otherwise, it is deleted as not helpful. In this case, clusters with identification cardinality < 50 were deleted. The final result is 3 clusters with identification cardinalities ≥ 230 .

$$H(X) = \sum_{i=1}^n p(x_i) \log_2 \frac{1}{p(x_i)} = - \sum_{i=1}^n p(x_i) \log_2 p(x_i),$$

$$\text{where } p(x_i) = \frac{|N_\varepsilon(x_i)|}{\sum_{j=1}^n |N_\varepsilon(x_j)|} \text{ and } n = num_{ln}$$

Figure 5.6: The entropy formula.

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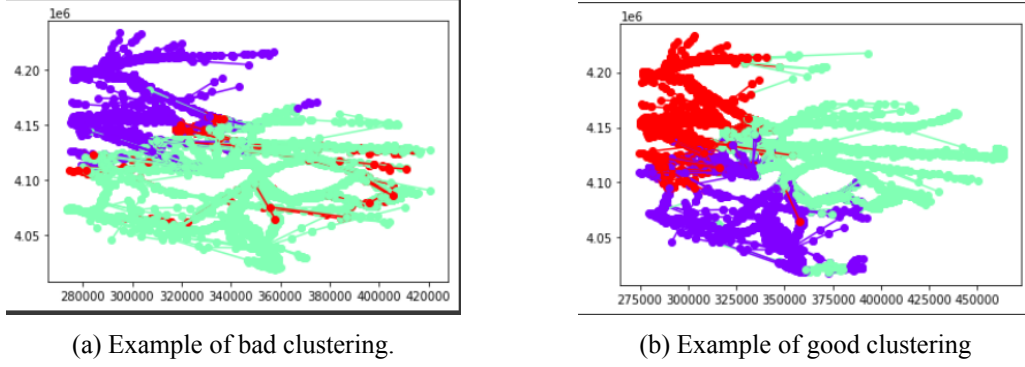


Figure 5.7: An intuitive example of good and bad quality clustering.

5.3 Representative Trajectories of the Clusters

Having acquired the clusters, the next step is to create their representative trajectories. With a set of vectors, the first step is to calculate the average direction vector, rotate the plane axes, and use a sweeping vertical algorithm that calculates the mean of the vectors it penetrates and their population. The average direction vector is given by the formula:

$$\vec{V} = \frac{\vec{u}_1 + \vec{u}_2 + \vec{u}_3 + \dots + \vec{u}_n}{|N_{u_n}|} \quad (5.2)$$

Having acquired the average vector, the X, Y axes are rotated until the average vector becomes parallel to the X axis. The angle ϕ of rotation between the average vector and the X axis can be extracted by the inner product of \vec{V} and the unit vector \vec{x} and the new coordinate system is given by the rotation matrix formula:

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = \begin{bmatrix} \cos(\phi) & \sin(\phi) \\ -\sin(\phi) & \cos(\phi) \end{bmatrix} \times \begin{bmatrix} x \\ y \end{bmatrix} \quad (5.3)$$

Having rotated the X, Y axes, the representations of all the vectors in the X', Y' are calculated in order to be used for the line sweep algorithm.

5.4 Applying the line sweep algorithm

The line sweep algorithm will be applied to the transformed vectors of the X', Y' plane. Since the plane was calculated in order for the X' axis to be parallel to the average vector, the line sweep

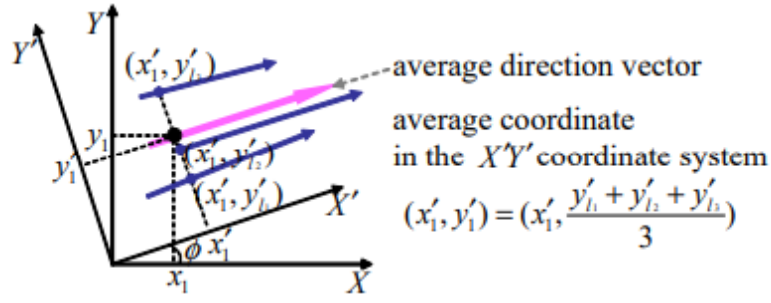
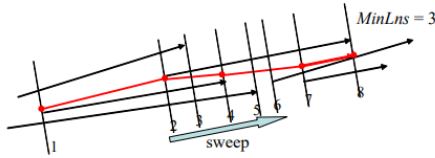


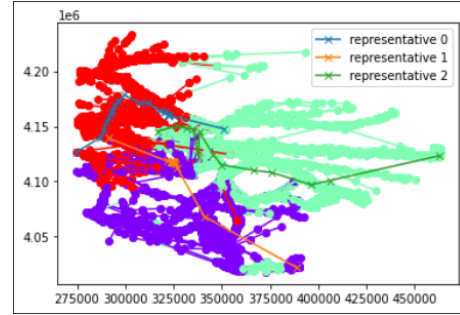
Figure 5.8: Example of the average vector \vec{V} and the rotation of the axes..
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will be applied with a line parallel to the Y' axis. For every step the algorithm moves the line in the X' axis, the population of the vectors it intercepts is counted; if the population is greater than a scalar number, the mean value Y' of the vectors and the algorithm's line X' value are assigned as a characteristic point. At the end, the trajectory created from the characteristic points is rotated back to normal, and the characteristic trajectory is extracted.



(a) Example of the sweep algorithm creating a characteristic trajectory.

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(b) The representative trajectories of the clustered data.

Figure 5.9: Extracting representative trajectories from data with the line sweep algorithm.

6. Training the Neural Network model with clustered data

Up until now, the sequence of actions has been as follows. Firstly, the representative trajectories of the real data were created using the MDL principle and distance function, then the hyperparameters ϵ and $MinLns$ were calculated using the entropy formula discussed in 5.5..2, and a density based algorithm for line segments, Traclus, was applied. Lastly, having created the clusters, the representative trajectory of each cluster was calculated using a sweep line algorithm. To train the neural network with clustered data, every row of the dataset has to be clustered accordingly. This can be accomplished in numerous ways. For this study, the representative trajectory points were interpolated, and the data were clustered based on the Euclidean distance between the points of the dataset and the cluster representative trajectories; if it was needed, extrapolation instead of interpolation was used. The dataset rows were assigned to the closest cluster by majority rule. The

training process was the same, as mentioned in Chapter 5.3. The results will be shown in Chapter 6.

Chapter 6

Results and analysis

Considering the results of the unclustered data, a difference in accuracy can be observed when the model is trained with a cost function of MAE compared to MSE. In general, the model trained with the MAE cost function yielded better results by up to 40 metres. In the cases where the MAE function underperformed, it can be explained by the lack of instances. In regards to the clustered data, better results are clearly observed. Regarding the choice between a model with MAE cost function compared to MSE, there is no significant difference in results, but it should be noted that in training, the MAE model weights were adjusted one to five epochs faster compared to the MSE model, making it a better overall choice.

Table 6.1: The mean euclidean distance between predicted and real positions of the unclustered data in time windows of 1 minute for the model trained with the cost function MAE compared to MSE.

Time window in minutes	distance in km (MAE)	distance in km (MSE)	number of observations
[0,2)	0.48	0.52	159
[2,3)	0.76	0.78	15024
[3,4)	1.14	1.17	5535
[4,5)	0.66	0.70	228
[5,6)	1.26	1.28	96
[6,7)	1.32	1.35	48
[7,8)	1.90	1.95	42
[8,9)	1.22	1.25	59
[9,10)	1.46	1.57	45
[10,11)	1.52	1.55	42
[11,12)	1.31	1.24	39
[12,13)	1.30	1.39	35
[13,14)	1.18	1.21	27
[14,15)	1.42	1.51	41
[15,16)	1.56	1.60	18
[16,17)	2.42	2.43	24
[17,18)	2.53	2.52	16
[18,19)	1.09	1.09	9
[19,20)	1.12	1.12	11
[20,21)	2.61	3.09	9
[21,22)	3.47	3.48	12
[22,23)	4.31	4.34	11
[23,24)	1.92	1.88	14
[24,25)	1.66	1.62	8
[25,26)	1.40	1.54	5
[26,27)	1.24	1.24	9
[27,28)	2.15	1.64	6
[28,29)	3.67	3.52	7
[29,30]	3.40	3.46	6

Table 6.2: The mean euclidean distance between predicted and real positions of the cluster 0 data in time windows of 1 minute for the model trained with the cost function MAE compared to MSE.

Time window in minutes	distance in km (MAE)	distance in km (MSE)	number of observations
[0,2)	0.11	0.11	19
[2,3)	0.13	0.13	761
[3,4)	0.19	0.19	317
[4,5)	0.25	0.25	13
[5,6)	0.32	0.32	8
[6,7)	0.38	0.38	4
[7,8)	0.44	0.44	4
[8,9)	0.51	0.51	3
[9,10)	0.57	0.57	6
[10,11)	0.64	0.64	5
[11,12)	0.69	0.69	1
[12,13)	0.73	0.73	3
[13,14)	0.81	0.81	3
[14,15)	0.85	0.85	2
[15,16)	0.94	0.94	1
[16,17)	0.99	0.99	1
[17,18)	nan	nan	nan
[18,19)	1.10	1.10	1
[19,20)	nan	nan	nan
[20,21)	nan	nan	nan
[21,22)	1.27	1.27	3
[22,23)	nan	nan	nan
[23,24)	1.43	1.43	1
[24,25)	1.46	1.46	1
[25,26)	nan	nan	nan
[26,27)	nan	nan	nan
[27,28)	nan	nan	nan
[28,29)	1.73	1.73	1
[29,30]	nan	nan	nan

Table 6.3: The mean euclidean distance between predicted and real positions of the cluster 1 data in time windows of 1 minute for the model trained with the cost function MAE compared to MSE.

Time window in minutes	distance in km (MAE)	distance in km (MSE)	number of observations
[0,2)	0.11	0.11	9
[2,3)	0.13	0.13	2732
[3,4)	0.19	0.19	1098
[4,5)	0.25	0.25	15
[5,6)	0.32	0.32	7
[6,7)	0.40	0.40	4
[7,8)	0.46	0.46	5
[8,9)	0.52	0.52	19
[9,10)	0.57	0.57	7
[10,11)	0.62	0.62	12
[11,12)	0.69	0.69	5
[12,13)	0.74	0.74	2
[13,14)	0.81	0.81	2
[14,15)	0.86	0.86	5
[15,16)	0.93	0.93	3
[16,17)	0.98	0.98	3
[17,18)	1.04	1.04	2
[18,19)	nan	nan	nan
[19,20)	1.18	1.18	1
[20,21)	nan	nan	nan
[21,22)	1.30	1.30	2
[22,23)	nan	nan	nan
[23,24)	1.39	1.39	2
[24,25)	1.45	1.45	1
[25,26)	1.54	1.54	1
[26,27)	1.60	1.60	2
[27,28)	1.65	1.65	2
[28,29)	1.68	1.68	1
[29,30]	nan	nan	nan

Table 6.4: The mean euclidean distance between predicted and real positions of the cluster 2 data in time windows of 1 minute for the model trained with the cost function MAE compared to MSE.

Time window in minutes	distance in km (MAE)	distance in km (MSE)	number of observations
[0,2)	0.10	0.10	42
[2,3)	0.13	0.13	3473
[3,4)	0.19	0.19	1255
[4,5)	0.26	0.26	61
[5,6)	0.32	0.32	25
[6,7)	0.38	0.38	14
[7,8)	0.44	0.44	11
[8,9)	0.50	0.50	13
[9,10)	0.56	0.56	15
[10,11)	0.62	0.62	5
[11,12)	0.69	0.69	15
[12,13)	0.74	0.74	8
[13,14)	0.80	0.80	6
[14,15)	0.86	0.86	12
[15,16)	0.92	0.92	2
[16,17)	0.97	0.97	5
[17,18)	1.04	1.04	6
[18,19)	1.10	1.10	3
[19,20)	1.17	1.17	2
[20,21)	1.22	1.22	5
[21,22)	1.27	1.27	2
[22,23)	1.35	1.35	8
[23,24)	1.40	1.40	3
[24,25)	1.46	1.46	2
[25,26)	1.53	1.53	4
[26,27)	1.58	1.58	3
[27,28)	1.65	1.65	1
[28,29)	1.71	1.71	3
[29,30]	1.75	1.75	2

Table 6.5: Easting and Northing R2 MAEs and MSEs values from the model trained with MAE cost function.

	unclustered	cluster 0	cluster 1	cluster 2
Test Northing R2:	0.99	0.99	0.99	0.99
Test Easting R2:	0.99	0.99	0.99	0.99
Test Northing \sqrt{MSE} :	684.76	791.68	723.67	854.49
Test Easting \sqrt{MSE} :	924.72	1,147.73	745.32	901.47
Test Northing MAE:	428.32	583.12	490.99	619.84
Test Easting MAE:	589.35	744.80	574.98	673.04

Table 6.6: Easting and Northing R2 MAEs and MSEs values from the model trained with the MSE cost function.

	unclustered	cluster 0	cluster 1	cluster 2
Test Northing R2:	0.99	0.99	0.99	0.99
Test Easting R2:	0.99	0.99	0.99	0.99
Test Northing \sqrt{MSE} :	689.43	603.07	724.53	867.10
Test Easting \sqrt{MSE} :	932.49	1,533.25	1,314.51	919.93
Test northing MAE:	442.68	371.56	487.69	654.31
Test easting MAE:	625.27	419.35	552.49	717.60

Chapter 7

Conclusion

This study investigated the trajectory prediction problem in maritime transportation and explored the efficacy of predicting future locations using unclustered data for Neural Networks and applying trajectory clustering algorithms to the data before training. The results suggest that both methods are able to produce accurate predictions, and the use of clustered data can further improve the accuracy of the models. This improvement is the result of reducing the dimensionality of the data by clustering while also improving the ability of the neural network to identify and draw insights from the given data. Overall, this study is proof that trajectories can be clustered in order to improve the trajectory prediction of neural networks and be applied to maritime transportation. Although the advantages of trajectory clustering are made clear, it is noted that trajectory clustering requires additional preprocessing steps that are time and computationally consuming. Future research on this subject can use different distance formulas or apply changes to the distance formula used. Weather data such as temperature and wind speed can be used to further improve the results. Finally, the use of different Neural Networks such as the Long Short-Term Memory, Convolutional Neural Networks and Ensemble Networks can be applied. In conclusion, this study shows the potential for trajectory prediction using trajectory clustering and Neural Networks and calls for further research to explore the optimal approaches for maritime vessel prediction.

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