ELUCIDATING US IMPORT SUPPLY CHAIN DYNAMICS: A SPATIAL-TEMPORAL GRAPH NEURAL NETWORK APPROACH

by

NIKOLAY ARISTOV

Master of Applied Mathematics and Physics, Moscow Institute of Physics and Technology (2005)

and

ZIYAN LI

Bachelor of Arts in German Literature, East China University of Political Science and Law (2017)

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Signature of Author: ....
Department of Supply Chain Management
May 18, 2024

Signature of Author: ....
Department of Supply Chain Management
May 18, 2024

Certified by ....
Elenna R. Dugundji, Ph.D.
Research Scientist

Certified by ....
Thomas Koch, Ph.D.
Postdoctoral Associate

Accepted by ....
Prof. Yossi Sheffi
Director, Center for Transportation and Logistics
Elisha Gray II Professor of Engineering Systems
Professor, Civil and Environmental Engineering

Elucidating US Import Supply Chain Dynamics: A Spatial-Temporal Graph Neural Network Approach

by

Nikolay Aristov

and

Ziyan Li

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Abstract

To enhance understanding of congestion points at ports and provide visibility into the incoming goods flow into the USA, this study focuses on maritime ports, using several ports along the East Coast of the United States as case studies. Based on the Automatic Information System (AIS) data, containing a variety of vessel data throughout the maritime voyage collected via radio frequency, we found all points of ships congestion along the coast line of the USA by utilizing Density-based spatial clustering of applications with noise (DBSCAN) algorithm, we built several predictive models for the port congestion status of container ships.

Congestion status impacts the flow of goods, as it slows the movement of container ships carrying incoming commodities. We analyzed historical commodity flow data and predicted the containerized value and weight of imported commodities based on Harmonized System (HS) codes using eXtreme Gradient Boosting (XGBoost).

Employing quantitative AIS data analysis provides insights into port congestion dynamics and commodity flow trends, indicating the potential to improve port management and logistics visibility.

This project also proposes next steps, that will create additional value for stakeholders in the Supply Chain industry. This study contributes to both theoretical and practical applications in maritime logistics.

Capstone Advisor: Elenna R. Dugundji, Ph.D.
Title: Research Scientist

Capstone Advisor: Thomas Koch, Ph.D.
Title: Postdoctoral Associate

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Contents

Acronyms

AIS Automatic Information System. 2, 9–13, 18, 29

ARIMA Autoregressive Integrated Moving Average. 15, 23, 31, 39

DBSCAN Density-based spatial clustering of applications with noise. 2, 14, 16–18, 27, 28, 38

EBIT Earnings Before Interest and Taxes. 33, 34, 40

ETA Estimated Time of Arrival. 11, 13

FLOW Freight Logistics Optimization Works. 8

GNNs Graph Neural Network. 14, 19, 20

GRU Gated Recurrent Unit. 20, 21

HS Harmonized System. 2, 22, 23, 30

IMO International Maritime Organization. 17

LSTM Long Short-Term Memory. 4, 19, 27, 30, 44

MAE Mean Absolute Error. 25, 29, 30, 35, 39, 44

MAPE Mean Absolute Percentage Error. 25, 29, 30, 35, 39, 44

MMSI Maritime Mobile Service Identity. 9

RMSE Root Mean Squared Error. 25, 35, 39

SHAP Shapley Additive Explanation. 14

SMAPE Symmetric Mean Absolute Percentage Error. 25, 29, 30, 44

SOG Speed Over Ground. 27, 28

STAGCN Spatio-Temporal Adaptive Graph Convolutional Networks. 14

STGNN Spatial Temporal Graph Neural Network. 16, 17, 19, 27, 29, 30, 44

U.S. DOT U.S. Department of Transportation. 8

XGBoost eXtreme Gradient Boosting. 2, 14, 15, 25, 27, 30, 35, 39, 40, 44

Chapter 1

Introduction

1.1 Background and Motivation

With an increasing level of international cooperation, the vulnerability of supply chains to disruptions also grows. In the last few years, supply chains have been affected by several global events, such as the COVID-19 pandemic and the Suez Canal obstruction, which, in turn, led to interruptions in goods flows, increased volatility of demand and supply, and increased costs for all participants. To reduce the negative impact of future disruptions on supply chains in the United States and, also, to provide greater visibility of goods flows for key stakeholders to increase cooperation between them, on March 15, 2022, the Biden-Harris Administration and U.S. Department of Transportation (U.S. DOT) announced the launch of a major supply chain initiative, Freight Logistics Optimization Works (FLOW).

According to the U.S. DOT, "Freight Logistics Optimization Works (FLOW) team at the U.S. DOT aims to help industry participants develop better and more responsive operations strategies that will improve supply chain throughput and resilience by sharing global ocean logistics data" (The United States Department of Transportation, 2022). One of the integral parts of supply chain networks in the USA is ocean ports. Ports are critical nodes in international trade and global supply chain networks. Every US$ of trade flowing through a port will directly or indirectly generate an additional US$ 4 of global industry output (Verschuur et al., 2022). Moreover, the ports are major entry points for imported containers arriving in the USA. Therefore, it is impossible to achieve a reasonable level of visibility without having the necessary information about logistics in ports, including visibility of the quantity and timing of goods flows.

1.2 Problem Statement and Research Questions

To increase the resilience of the nationwide supply chain network, it is necessary to have a better understanding of the processes at the most upstream part of goods flow in the USA – the ocean ports. This understanding will give information about the estimated arrival time of goods, as well as their category, quantity, and routing. The information obtained may then be used by stakeholders for better planning of transportation, allocation of resources, and ordering and sourcing of goods.

The initial problem can be split into two major parts. The first part of the problem is the prediction of port congestion, which will give us an estimation of the goods flow into the USA, possible delays, and the possibility to re-route flows. In this part, we will deeply study the Automatic Information System (AIS) data, and select and compare different statistical or machine learning models to predict berth occupation, time spent by ships at the berth, and time spent waiting for berthing. The AIS collects vessel data throughout the maritime voyage via radio frequency, improving safety and traceability in global ocean logistics. The data includes Maritime Mobile Service Identity (MMSI), which is an identification number for each vessel; dynamic geographical data, such as longitude and latitude, that makes it possible to track the path (trajectory) of ships in the ocean; and static vessel information, such as length and beam (Yang et al., 2019). The International Maritime Organization's International Convention for the Safety of Life at Sea requires AIS to be fitted aboard international voyaging ships with 300 or more gross tonnage, and all passenger ships, regardless of size (International Marine Organization, 2004). Besides the use of historical AIS data for estimating port congestion and time spent by container ships on berth or prior to entering the port, we have to consider other exogenous factors, such as delays at the transshipment ports, congestion near the port, and supply chain disruptions during pandemics or strikes, which may affect the accuracy of the port's operations predictions. We researched the influence of these factors on the prediction model.

The second part of the problem is to analyze the goods flowing through the port. There could be level, trend, and seasonality in the underlying model of goods flow; knowing these parameters and their interrelationships will provide good visibility for all the stakeholders in the downstream goods flow.

In that context, the research questions to be answered include:

1. What analytics could be useful for all stakeholders to increase the resilience of supply chains and the visibility of import flows?

    (a) What factors affect the type of goods imported via our principal port of study, the Port of Boston?

    (b) What is the effect of exogenous factors on congestion and goods flow prediction?

1.3 Project Goals and Expected Outcomes

Our project focuses on the container terminals of the ports on the East Coast of the USA (the full list of ports is presented in Table A.1). The aim of the project is to perform a spatial-temporal analysis of the supply chain dynamics of global ocean logistics networks. Additionally, it targets developing descriptive and predictive models of the congestion of the ports in the scope, and of the goods flow imported through the Port of Boston.

First, we identified the key elements and drivers of ocean networks that affect the congestion of ports. In this research, we worked with the AIS data, in which the timestamps along with coordinate points of vessels can help us get an insight into the routes of vessels crossing the ocean and the actual time spent at the port and premises.

AS part of the work we also retrieved past actual routes from AIS data. Moreover, the AIS data gave us insider information about other points to consider in our models, such as straits, channels or artificial obstacles on the route, that are impacting traffic flow.

As shown in Table 1.1, the AIS collects a variety of vessel data via radio frequency at regular intervals throughout the voyage.

Table 1.1

Automatic Information System (AIS) Data Information

Field Name	**Description**
MMSI	Maritime Mobile Service Identity, unique nine-digit identification number for each vessel
BaseDateTime	Date and time of the AIS signal
LAT, LON	Geographical coordinates of the vessel
SOG	Speed over ground in knots
Draught	Draught of ship
COG	Course over ground in degrees from true north
IMO	IMO ship identification number, a unique and permanent seven-digit identification number
Static data	Length, width, draft, etc.

Additionally, the U.S. Census Bureau's data on import trade provides clear information on goods imported into the US. We used the data for the Port of Boston to analyze the goods categories and seasonality. Mapping the goods flow imported to the Port of Boston to the Estimated Time of Arrival (ETA) could give stakeholders a clearer view of ocean logistics and networks.

We built and compared several methodologies, such as statistics, machine learning and neural network models, to provide a model with the highest accuracy. Moreover, we changed the input into the model to check different scenarios' impact on the model.

The deliverables of this project include:

1. Prediction models of the berth occupation of the terminals in the ports under consideration.

    (a) Time spent by container ships on berth and on premises.

2. Descriptive and predictive models of goods flow through the Port of Boston.

3. Scenarios simulation of possible incidents of a pandemic, strikes, or other restrictions that impact the congestion and berthing time of the ships and goods flow.

1.4 Performed Works

To achieve the project's goals, we completed the following tasks:

Prediction models of the berth occupation of the terminals in the ports under consideration.

1. Specified the input information required for the building of the predictive model of port' congestion.
2. Cleaned the AIS, Census and other datasets.
3. Built a list of potential exogenous factors affecting prediction.
4. Built different models for the congestion prediction and compared them:
   (a) Statistical models
   (b) Machine learning models
   (c) Neural Networks

Descriptive/Predictive Model of goods flow

1. Specified the input information required for the building of the descriptive/predictive model of goods flow.
2. Selected Census data for the Port of Boston at the monthly, quarterly, and yearly levels.
3. Built different models for the goods flow and compared them:
   (a) Statistical models
   (b) Machine learning models
   (c) Neural Networks

Chapter 2

State of the Practice

In recent research projects, several studies have delved into predicting vessels' behaviors, addressing challenges related to congestion and traffic flow, and optimizing port operations. Also, besides statistical models, more advanced methodologies have been applied in transportation research, such as Neural Networks and Transformer, which show promising results in predicting ETA. In this section, literature regarding these areas will be discussed.

2.1 Prediction of Port Congestion

As described in Section 1.2, the problem of congestion prediction could be separated into several parts. At first, we have to understand the layout of the maritime network. Then we continue with works on the prediction of traffic congestion and modeling of the port's operations in the immediate vicinity of the port. We also research articles predicting the congestion of other modes of transportation, such as trains or truckloads, which also give us insights on how to make predictions using different methods.

2.1.1 Traffic Congestion

The ability to find congestion points and predict traffic flow is crucial for accurate ETA predictions. Analyzing historical AIS data allows us to identify anchor and berth areas of the port by utilizing a specially developed algorithm based on the Density-based spatial clustering of applications with noise (DBSCAN) method (Bai et al., 2023). This algorithm was tested on eight ports with complicated geographic features and could be an appropriate starting point for the analysis of port ecosystems. The algorithm itself could also be used for monitoring congestion data at the specified ports. We utilized this algorithm to receive initial information about the maritime network layout.

T. Zhang et al. (2023) showed that eXtreme Gradient Boosting (XGBoost) and Shapley Additive Explanation (SHAP) could be used to predict port congestion status and improve the prediction accuracy of time spent in port. It was also stated that for predicting the traffic flow rate, the XGBoost algorithm had the lowest error for hour-ahead forecasts in comparison to Holt-Winters, Transformer, and Graph Neural Network (GNNs) (Belt, 2023). We will use this algorithm as a benchmark to compare it with our target model.

Ma et al. (2023) used Spatio-Temporal Adaptive Graph Convolutional Networks (STAGCN) to extract the properties of the road network topology graph. First, the authors captured the structure of the road network traffic by using an adaptive graph generation block, built an adaptive road network topology graph, and then fed the result to capture spatial-temporal features of the traffic data by utilizing spatial-temporal convolution blocks. This work tested the approach on publicly available datasets for freeway traffic and claimed that prediction accuracy outperformed modern baseline methods. However, the authors stated that STAGCN has limitations, as it requires two features: traffic flow and traffic speed.

We built our model based on the work of Wang et al. (2020). The work proposes the utilization of a spatial temporal graph neural network for traffic prediction. This algorithm can capture comprehensive spatial data, which is necessary in the maritime network of the East Coast of the USA, where two major ports, New York / New Jersey and Savannah, affect traffic and goods flow in the rest of the East Coast ports. This model also captures temporal patterns by capturing sequential components.

2.2 Analysis of Commodities

A comprehensive understanding and prediction of incoming commodities are pivotal for the operation and development of a seaport, enabling the port to enhance the berth operation with clearer insights into the weight and value of incoming commodities. The weight of commodities directly impacts the port's operations, such as crane allocation, berth schedules, and warehouse storage requirements. On the other hand, the value of commodities could influence operation prioritization and customs clearance. Forecasting for both weight and value is essential for the strategic allocation of port resources.

With limited data, time series models such as Holt-Winters and Autoregressive Integrated Moving Average (ARIMA) are common methods to provide a promising prediction of the value and weight of incoming commodities. However, the supply chain disruption during the pandemic made the statistical models difficult to use to provide accurate predictions. More advanced machine learning models are required to apply to forecasting the value and weight of imported commodities. Several machine learning methods are introduced to predict future trade trends, such as XGBoost (Batarseh et al., 2019).

Furthermore, feature engineering is a necessary aspect of developing machine learning models, influencing their performance and effectiveness. In addition to the historical data on the commodities themselves, multiple exogenous factors have been introduced that could influence the future trends of trade, such as product ranking and inventory gross margin return on investment (T. Zhang et al., 2023). This research compared several machine learning models incorporating these features, aiming to predict quantities of goods to be imported.

We used and compared Holt-Winters, ARIMA, boosted hybrid model, and XGBoost with different input features for forecasting commodities' value and weight.

Chapter 3

Methodology

In this chapter, the methodology used to conduct the research for the project is described. We started with steps to build prediction models of congestion of the port and ended with modelling of flow of commodities.

3.1 Introduction

We approached the prediction of congestion of ports in several steps. First, we identified areas for the scope of our work, such as terminals, ports, waiting areas, and congestion points, as an output of the DBSCAN algorithm. This gave us valuable information about the maritime network layout along the US coastline. This also allowed us later to build a graph for our Spatial Temporal Graph Neural Network (STGNN) network.

We built several statistical models for predicting berth occupation in several terminals and ports, as well as the number of container ships in the waiting area. This gave us a benchmark for our STGNN model's performance.

Next, we built, trained and tested our STGNN model, then analyzed the results and proposed next steps to increase the value of the model for the stakeholders.

As the last step, we described the imported commodities' time series features and used the predicted berth occupation as a parameter for predictive models of the flow of commodities imported through the Port of Boston.

3.2 Constructing the Network

In this section, we describe our approach for detecting and describing points of interest and creating nodes for the graph of the STGNN model.

3.2.1 Data Handling

We used AIS data for container ships in the vicinity of the coastline of the USA for the years 2015 through 2023, filtered by the International Maritime Organization (IMO) number of container ships.

3.2.2 DBSCAN

Density-based spatial clustering of applications with noise is a data clustering algorithm introduced by Ester et al. (1996). Density-based spatial clustering of applications with noise (DBSCAN) detects clusters of high density and treats areas of low density as noise. This algorithm is useful as it does not require specifying a number of clusters; therefore, it is able to find all points of interest. The algorithm relies only on two parameters: the minimum number of points to form a cluster and the radius of a neighborhood with respect to some point. A cluster in DBSCAN consists of a set of core samples (which are neighbors to each other) and a set of non-core samples that are neighbors of these core samples.

To narrow our research, we filtered data by speed over ground, assuming that ships in anchorage and berth areas are spending some time with drift speed or on full stop (berthed, anchored).

3.2.3 Addressing Ship Positions

For the purpose of our models and detecting ship positions, we applied several techniques for different areas and points of interest:

1. Berthing: Some of the ports (for example, Los Angeles/Long Beach, New York/New Jersey) have several terminals situated closely to each other and

a complicated geometry of the berth. To address this issue, we constructed a multi-line with coordinates of the points at the beginning and end of each terminal's berth and, also, points where the orientation of the berth changes. We assumed that ships were berthing if the distance to the nearest sector of the line was less than 60 meters. Since the heading data in AIS is sometimes not reliable and the message frequency and time of berthing are smaller compared to the time discrepancy of the model, which is one day, we assumed that this is a good approximation of the ship being berthed.

2. Waiting (Anchorage) area: This area is a polygon, surrounding a manually identified and classified cluster, that was detected by the DBSCAN algorithm. All container ships that appeared inside the polygon were counted toward the total number of vessels that spent some time in the area prior to entering the port.

3. Harbor area: This area is a manually identified polygon, encompassing the water area from the entrance to the harbor and all areas of the harbor that are open to container ships, including terminals.

3.2.4 Building Features

To generalize the model, we analyzed the list of container ships that visited ports in the USA. We split them into categories of operators, grouping them by major operators (having more than 10 ships) to correspond with the terminals preferred by each operator; the rest of the ships were considered in one group. We also grouped ships by size (length and width). For grouping by size, we performed clustering by applying k-means clustering (Lloyd, 1982). Apart from generalization, this allowed us to decrease the number of features and make computations easier. For our models, we used a 7-day history for the number of ships in the particular node and the number of ships heading to the node. We also used date data, such as the month and day of the week.

3.3 Statistical and Machine Learning Models

We built several models to predict the berth and anchorage areas' occupation for terminals based on historical occupation. These models could be used as a benchmark for the STGNN model.

3.3.1 Random Forest Regression

Random Forest, or Random Decision Forest, is a method to perform classification or regression by constructing and combining multiple decision trees. This method was introduced by Ho (1995).

We applied these methods to predict congestion at every terminal in the scope of our work.

3.3.2 Long Short-Term Memory (LSTM) Networks

Long Short-Term Memory (LSTM) Networks are one of the most widely known and commonly used methods for dealing with time series, as introduced by Hochreiter and Schmidhuber (1997). This technique is commonly used for forecasting and is well documented. More information can be found in Staudemeyer and Morris (2019).

We applied this method to predict congestion at all modeled terminals.

3.3.3 XGBoost

This method is discussed in Section 3.5.5 We applied this method to predict congestion at all modeled terminals.

3.4 Spatial Temporal Graph Neural Network

For the purpose of this work, we used the Spatial Temporal Graph Neural Network (STGNN). This is a subclass of the more general class of Graph Neural Network (GNNs), which are used to predict traffic intensity due to their ability to utilize spatial information. The framework for our model was proposed by Wang et al. (2020) and was used to predict road traffic.

3.4.1 Layers

The framework consists of four layers: a GNNs layer to capture spatial information, a Gated Recurrent Unit (GRU) layer to capture local temporal dependencies, a transformer layer to capture global temporal dependencies, and a multi-layer feed-forward network to output predictions.

Graph Neural Network Layer

For modeling spatial dependency, the framework used the Graph Neural Network Layer:

$$X_{out} = f(\widetilde{D}^{-1/2}\widetilde{A}\widetilde{D}^{-1/2}X_{in}W)$$

where f is a non-linear activation function, allowing it to capture more complex patterns; and matrix W contains the parameters to be learned.

For the purpose of our work, we used $\widetilde{A}$ as the refined adjacency matrix, defined by equation:

$$\widetilde{A} = A + I_N$$

where A is the adjacency matrix that maps the connections between nodes; and I_N is the N-dimensional identity matrix. We defined adjacency matrix A as:

$$A_{ij} = \begin{cases} \exp(-d_{ij}^2/\sigma^2), \text{ if } i \neq j \\ 0, \text{ otherwise} \end{cases}$$

where d_{ij} is a distance between two nodes (see definition of nodes in section 3.4.2); and σ is the standard deviation of the distances. Lastly, we have the refined degree matrix:

$$\widetilde{D}_{ii} = \sum \widetilde{A}_{ij}$$

Gated Recurrent Unit Layer

This layer is used to capture temporal dependencies. GRU was introduced by Cho et al. (2014). This layer applies to each node individually and the parameters of GRUs for all the nodes are shared with each other. The GRU operation at time t for node v_i can be expressed as:

$$z_t = \sigma_z(W_z \widetilde{X}_t[i,:] + U_z \widetilde{H}_{t-1}[i,:] + b_z),$$

$$r_t = \sigma_r(W_r \widetilde{X}_t[i,:] + U_r \widetilde{H}_{t-1}[i,:] + b_r),$$

$$\widetilde{H}_t[i,:] = \tanh\left(W_h \widetilde{X}_t[i,:] + U_h(r_t \odot U_h \widetilde{H}_{t-1}[i,:]) + b_h\right),$$

$$H_t[i,:] = (1 - z_t) * \widetilde{H}_{t-1}[i,:] + z_t \odot \widetilde{H}_t[i,:].$$

where $\odot$ is the element-wise multiplication, W_z, W_h, U_z, U_r, U_h are the parameters to be learned and $H_t[i,:]$ is the output of the GRU layer and the hidden representation of the current time step. σ_z and σ_r are sigmoid functions.

Transformer Layer

The GRU layer models local temporal dependency. For our problem, temporal information should also be modeled globally. To deal with this, we utilized a transformer layer (Vaswani et al., 2017). This layer stacks all layers derived from the previous layer and applies transformations to the stacked matrix. Given that the transformer ignores the relative position in the sequence, we used positional encoding determined by

$$e_t = \begin{cases} \sin(t/10000^{2i/d_{model}}), \text{ if t} = 0,\ 2,\ 4... \\ cos(t/10000^{2i/d_{model}}), \text{ otherwise.} \end{cases}$$

This gives us

$$H'_t[i,:] = H_t[i,:] + e_t$$

Next, we applied a one-layered transformer-based encoder with a normalization layer to the encoder's inputs.

The output of the transformer layer was used as the input of the Prediction Layer.

Prediction Layer

As a final layer, we used a multi-layer feed-forward network. This network uses the output $H_{out}^{v_i} | v_i \in V$ of the transformer layer to make predictions for the number of ships at nodes.

3.4.2 Building the Graph Neural Network

For our model, we used three types of nodes:

1. Ports
2. Waiting zones of ports
3. Terminals in ports

Ports represent physical ports like Boston or New York and are connected by bidirectional edges. Each port is linked by a unidirectional edge to the port's waiting zone, which represents a zone where container ships could wait for berthing. The waiting zone, in turn, has a unidirectional edge to every terminal in port. Terminals in the port are connected bidirectionally to each other (representing the possibility of the ship using several terminals) and to the port node, representing entering and exiting the port. Edges are represented in the model by an adjacency matrix defined by the physical distance between nodes.

3.5 Predictive Models of Commodities through the Port of Boston

3.5.1 Data Handling

We began the analysis of commodities imported into the Port of Boston from the importation dataset by 2-digit Harmonized System (HS) code from 2003 to 2023.

The HS code is utilized by the World Customs Organization as a system of six-digit codes to categorize commodities (Pierce & Schott, 2012). We selected the top five commodities by filtering containerized value and weight, in order to capture the trend, seasonality and other nonlinear relationships and build predictive models.

3.5.2 Holt-Winters Exponential Smoothing

In the analysis of time series data, Holt-Winters is a common statistical approach for forecasting seasonality. In this study, we employ a Python package to automatically find the optimal combination of data, trend and seasonal smoothing factors.

The equations below show how the Holt-Winters model works (Winters, 1960):

$$\hat{x}_{t,t+\tau} = (\hat{a}_t + \tau \hat{b}_t)\hat{F}_{t+\tau-P}$$

$$\hat{a}_t = \alpha(\frac{x_t}{\hat{F}_{t-P}}) + (1-\alpha)(\hat{a}_{t-1} + \hat{b}_{t-1})$$

$$\hat{b}_t = \beta(\hat{a}_t - \hat{a}_{t-1}) + (1-\beta)\hat{b}_{t-1}$$

$$\hat{F}_t = \gamma(\frac{x_t}{\hat{a}_t}) + (1-\gamma)\hat{F}_{t-P}$$

where

x_t : Actual demand in period t

$\hat{x}_{t,t+\tau}$: Forecast for time $t + \tau$ made during time t

F_t : Multiplicative seasonal index appropriate for period t

P : Number of time periods within the seasonality

α : Data smoothing factor $\alpha \in [0, 1]$

β : Trend smoothing factor $\beta \in [0, 1]$

γ : Seasonal change smoothing factor $\gamma \in [0, 1]$

3.5.3 ARIMA Model

When facing non-stationary time series data, an Autoregressive Integrated Moving Average (ARIMA) model provides better performance than Holt-Winters. It is composed of the following models:

- Autoregressive models (AR) forecast a time series' future values based on its past value, assuming the current value is a linear function of its previous values plus a random error term.
- The integrated portion (I) is used to make the time series' values stationary.
- Moving average models (MA) forecast future values of a time series based on its past forecast errors, assuming the current value is a linear function of past forecast errors plus a random error term. (Hyndman & Athanasopoulos, 2018)

In this study, we used the Python package auto-arima to automatically determine the order of autoregressive terms, moving average terms, and seasonal AR, MA, and differencing parameters.

3.5.4 Boosted Hybrid Model

The Boosted Hybrid model is a hybrid approach that synergizes a linear regression model that discerns normal variables correlated with the target values, such as Fourier, lags, and leads, subsequently refining the prediction by training on the residuals with other exogenous or less common variables to capture the peaks or troughs within the dataset.

Given the highly oscillated historical data on imported commodities, we saw a great possibility of applying the boosted hybrid model to significantly enhance the precision of predicting the value and weight of imported goods.

In the context of linear regression, variables such as lags and specific holiday effects were considered. For example, we took Christmas as a one-hot encoded feature[1] to mitigate seasonal impacts on the observed data. We also delineated the unseasonalized data through its autocorrelation, partial autocorrelation, and lags, thus enabling a clearer analysis.

[1] One-hot encoded feature is a widely-used method of transferring categorical variables to binary vectors.

After calculating the residuals from the first model, we applied the RandomForest model to train the residuals by features such as month of year and holiday months.

3.5.5 XGBoost

eXtreme Gradient Boosting (XGBoost) presents a scalable and efficient solution for tree ensemble learning, consisting of multiple decision trees to form robust predictive models. The XGBoost algorithm assigns scores of i-th leaf of each decision tree and sums up these scores for the corresponding leaves to achieve the final prediction. To optimize the performance of the model, XGBoost minimizes the following regularized objective function (Chen & Guestrin, 2016):

$$\mathcal{L}(\phi) = \sum_i l(\hat{y}_i, y_i) + \sum_k \Omega(f_k)$$

$$\Omega(f) = \gamma T + \frac{1}{2}\lambda \|w\|^2$$

where

l : a differentiable convex loss function that measures the difference between actual data y_i and prediction $\hat{y}_i$

Ω : penalty of the complexity of the model

f_k : function corresponding to an independent tree structure and leaf weights w

T : the number of leaves in the tree

λ : additional regularization term smoothing the final learned rate to avoid overfitting

3.6 Error Measures

To evaluate the performance of commodity models, Mean Absolute Percentage Error (MAPE), Root Mean Squared Error (RMSE) and Mean Absolute Error (MAE) have been applied. The smaller the values are, the better the performance is. For congestion models we utilized Symmetric Mean Absolute Percentage Error (SMAPE), as it works better with series due to having a lot of 0 and 1 values.

$$MAPE = \frac{100\%}{N}\sum_{i=1}^{N}|\frac{y_i - \hat{y}_i}{y_i}|$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}$$

$$MAE = \frac{1}{N}\sum_{i=1}^{N}|y_i - \hat{y}_i|$$

$$SMAPE = \frac{100}{n}\sum_{i=1}^{N}\frac{|F_t - A_t|}{(|A_t| + |F_t|)/2}$$

Chapter 4

Results

This section is dedicated to the results of the statistical and machine learning models we built to meet our research objectives.

Initially, DBSCAN was employed to categorize areas based on density. Then Random Forest Regressor, LSTM, XGBoost and STGNN were applied to predict the number of vessels in each area. We also explored statistical models, boosted hybrid models and XGBoost to predict the containerized value and weight of imported commodities.

We present the outcomes and findings derived from these models.

4.1 Congestion Points

We performed initial clustering by utilizing the DBSCAN algorithm for the AIS data set, which contains data about ships' movements along the US coastline for the period from January 1, 2015, to September 30, 2023. We filtered the original data only by container ships and Speed Over Ground of less than 5 km per hour (meaning, that a ship could drift with a flow and not be anchored). This clustering limited the set of points we needed to consider for building our model. We started the algorithm by using a radius of 10 km and a minimum sample size of 100 as parameters. This allowed us to identify all container ship ports along the US coastline. However, it didn't allow us to have more detailed information. We also saw that we should reduce the radius for the detection of port terminals in complicated areas. By decreasing these numbers to 2 km and 100, we were able to identify all terminals in New York / New Jersey ports, for example, but we still needed more precise clustering for ports with complicated berth geometry and narrow separation of terminals (for example, Los Angeles/ Long Beach). However, the analysis identified all ports with container terminals in the USA and congestion points such as, for example, the bridge near Annapolis on the way to the Port of Baltimore. We could also clearly see increasing and decreasing congestion in ports over time.

By performing statistical analysis of AIS data for the Boston port area (berth, anchorage areas), we observed no seasonal or time effect. We confirmed with port authorities that the only reason, except for some unrelated to the port (like technical issues or rescheduling), for ship timing in the wait area is traffic inside the harbor.

By performing initial clustering with parameters (SOG/Number of Vessels/Radius km) and plotting the centroid of clusters onto a map, we identified points of interest for our research. We were also able to see an increase in the density of such points in 2021-2022, which corresponds to the actual situation with container ships around the USA. Points of interest identified could be split into three major groups:

1. Waiting zone area – the area outside the port where ships could spend several hours before entering the port area.

2. Port/berth area – actual mooring (berthing) points

3. Points in front of an obstacle in the way of a ship, like a bridge or channel. While these points are not directly related to port activities, they could cause a delay for the vessel en route.

While we were not able to confirm with authorities that the waiting area identified is officially designated as an anchorage, it can serve as an initial proxy to collect historical data on ships entering the waiting pattern. DBSCAN clustering provided good identification of the berth area. However, in ports with challenging geometries, like New York/New Jersey and Los Angeles/Long Beach, it is complicated to identify a specific terminal for the ship. The analysis of AIS data showed that relying on the status of the ship field is also not feasible, as there are many cases when the crew forgot to switch it from one status to another.

To approach the problem of vessel berth identification, we chose points at the end of each berth and the change in geometry of each terminal/port included in this work. Apart from coordinate identification, this gave us the direction (heading) of the berth. By using both coordinates and headings, we were able to identify the mooring of ships by calculating the distance between the ship and berth line and comparing the heading of the ship with the berth direction. The analysis of AIS data showed that some of the ships have problems transmitting the correct heading, so our approach is to detect the start time and end time of berthing by filtering ships with a distance less than the width of the ship berthing. We assume the possible error is not more than 10-15 minutes, which is not affecting our model, as we have a discrepancy of 1 day.

4.2 Congestion Prediction Models

We built several models for the terminals under consideration to predict congestion at them. These models were used as benchmarks for our Spatial Temporal Graph Neural Network model. As an input for the models, we used the number of vessels at the berth per day at terminals, the number of ships heading to the particular terminal from other terminals in the model in the last 7 days, and, additionally, time series categories like month and day of the week. As an output, we predicted the number of vessels in terminals. By analyzing benchmarking models, we used such error metrics as MAE, MAPE and SMAPE.

Although Random Forest Regression achieved the smallest prediction error, the features it relied on appear to have no meaningful relationship with the predicted outcomes. In this case, the chosen features shared coincidentally similar values with the target variable, leading to misleadingly low error rates. Therefore, we excluded this model from comparison.

The comparative results of all methods by terminal can be found in Table A.2.

The Table 4.1 displays three different terminals with different winning models. To understand this phenomenon, additional research into the differences between terminals and of incoming traffic should be conducted. This further study could reveal additional insights into improving the models.

Table 4.1

Errors by Terminals, Models

Port Terminal	Model	MAE	MAPE	SMAPE
APM Terminals	LSTM	1.57	37.64	47.08
	STGNN	1.52	55.16	41.05
	XGBoost	**0.52**	**12.28**	**12.82**
Port Liberty Bayonne Terminal	LSTM	0.70	50.68	84.62
	STGNN	**0.51**	**37.75**	**45.18**
	XGBoost	0.67	58.92	54.50
The Red Hook Container Terminal	LSTM	**0.36**	**57.94**	158.42
	STGNN	1.39	79.62	147.71
	XGBoost	0.94	72.32	**146.14**

Note. In bold shown the best error per terminal

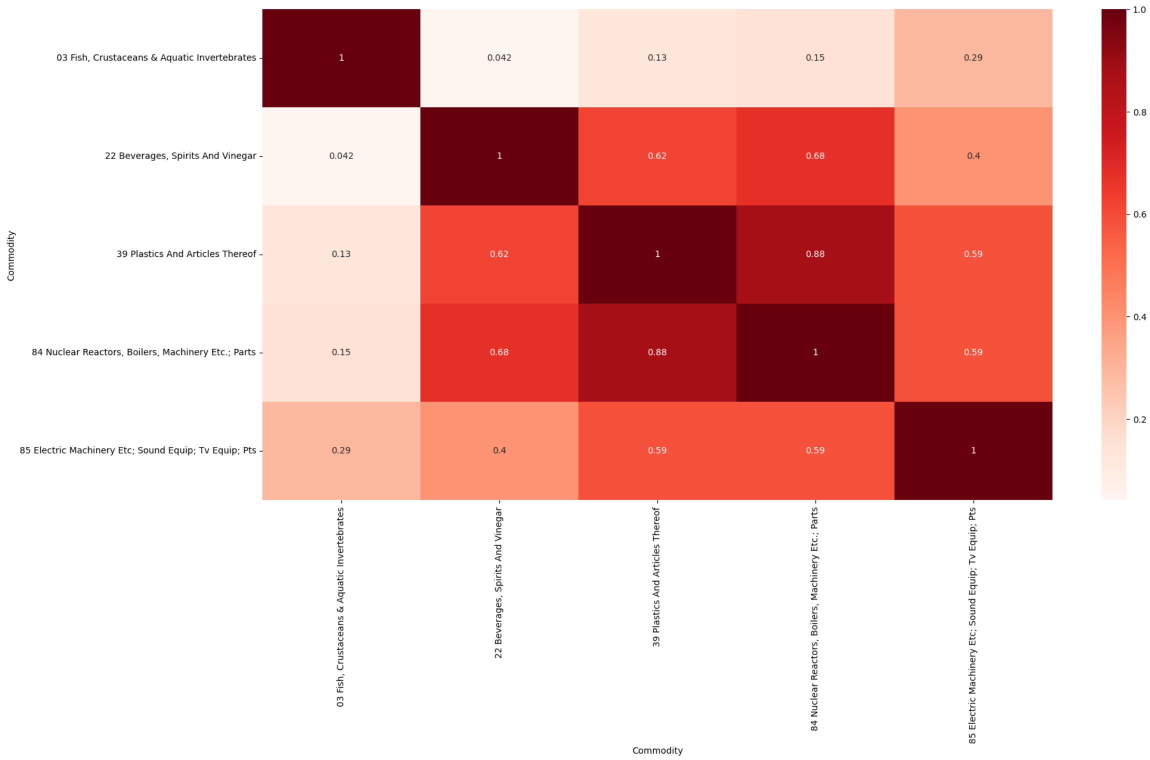
4.3 Commodities

Based on the import data by 2-digit HS code from 2003 to 2023, we first took a look at the five highest-value commodities imported during that period by the Port of Boston. The most valuable commodity (total containerized value in USD) during the past 20 years was identified by HS Code 84 (Nuclear Reactors, Boilers, Machinery, Etc.). In the analysis of the targeted value, a heatmap revealed a pronounced correlation between commodity 84 (Nuclear Reactors, Boilers, Machinery, Etc.) and commodity 39 (Plastics And Articles Thereof) with a pairwise correlation coefficient of 0.88. The heatmap 4-1 graphically shows the interrelationship among the observed variables.

After communication with Port of Boston, it emerged that within the Boston area, the observed strong correlation between commodities classified by HS code 84 and 39 may stem from their use in the medical sectors, such as medical laboratory equipment,

Figure 4-1

Heatmap of Value Correlation Coefficient



dialysis machines, plastic labware or plastic components for medical devices. This correlation is likely influenced by the demand from hospitals and medical facilities. So, we decided to aggregate these two commodities to see a general feature.

On the other hand, the commodity with the highest weight, classified under HS Code 22 (Beverages, Spirits, and Vinegar), has exhibited a stable trend and clear seasonality over the past 20 years. We utilized these two datasets as case studies to elucidate the analytical outcomes.

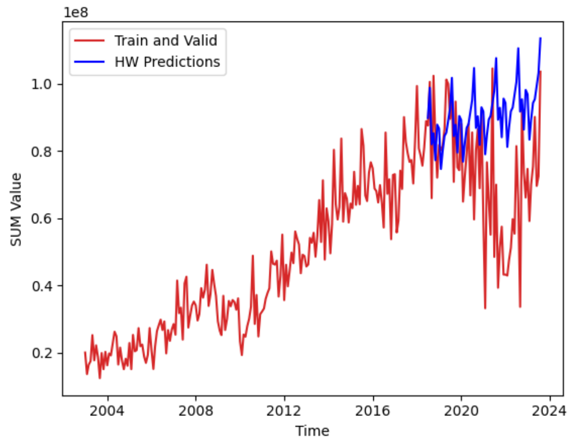
4.3.1 Statistical Models

We employed Holt-Winters and Autoregressive Integrated Moving Average (ARIMA) methodologies to analyze the time series data. The data was partitioned into 75% for training and 25% for testing. Figure 4-2 and Figure 4-3 demonstrate the robust outcomes of the Holt-Winters and Auto ARIMA models, with the red line depicting actual data and the blue line representing predicted data.

Figure 4-2

Holt-Winters and Auto ARIMA models' Result of Sum Containerized Value of Commodity Identified by HS Code 84 and 39

(a) *Holt-Winters Model Result*



(b) *Auto ARIMA Model Result*

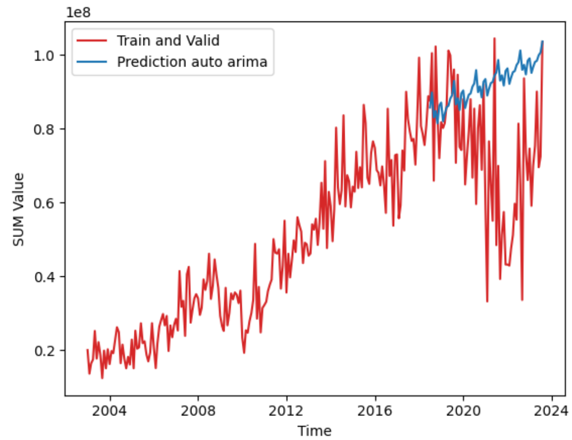
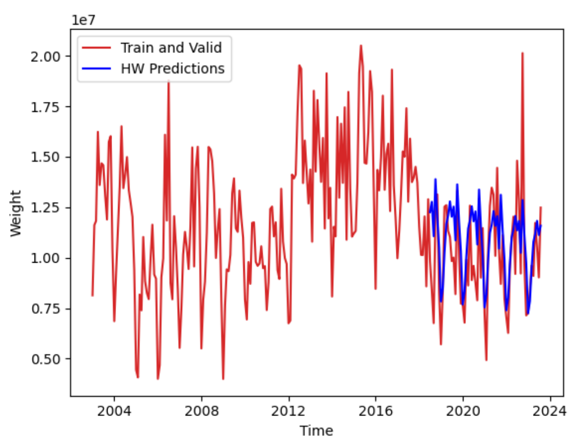


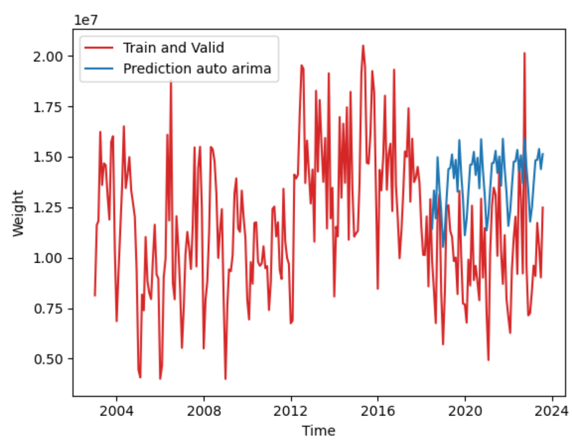
Figure 4-3

Holt-Winters and Auto ARIMA models' Result of Sum Containerized Weight of Commodity Identified by HS Code 22

(a) *Holt-Winters Model Result*



(b) *Auto ARIMA Model Result*

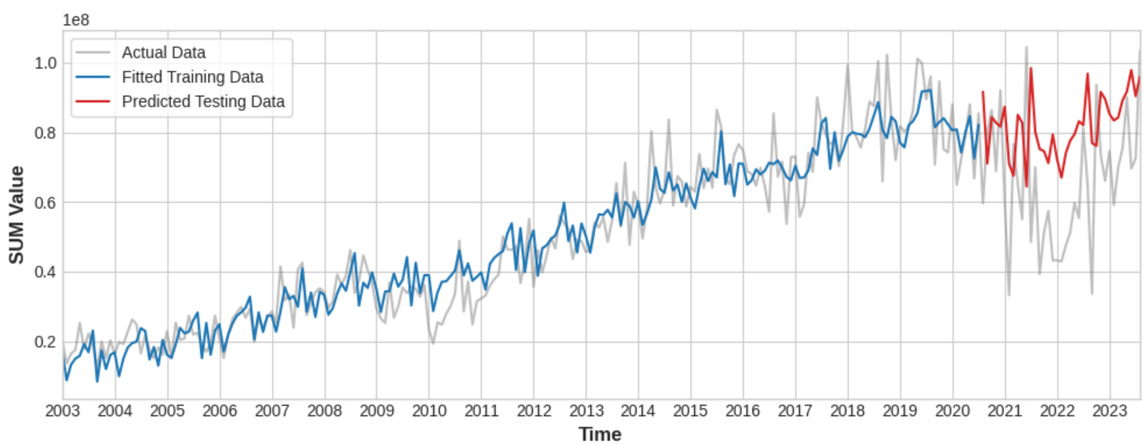


4.3.2 Boosted Hybrid

As described in Section 3.5.4, a two-tiered hybrid modeling approach comprised ridge regression for time steps and lagged variables, and a Random Forest Regressor to train on the residuals derived from the first model. As depicted in Figure 4-4, the boosted hybrid model yields relatively more accurate predictions for the sum containerized values of commodities 84 and 39, where the gray line denotes the actual data, the blue line indicates the training data, and the red line signifies the predictions for the testing data.

Figure 4-4

Boosted Hybrid Model for Aggregated Value of Commodity Identified by HS Code 84 and 39

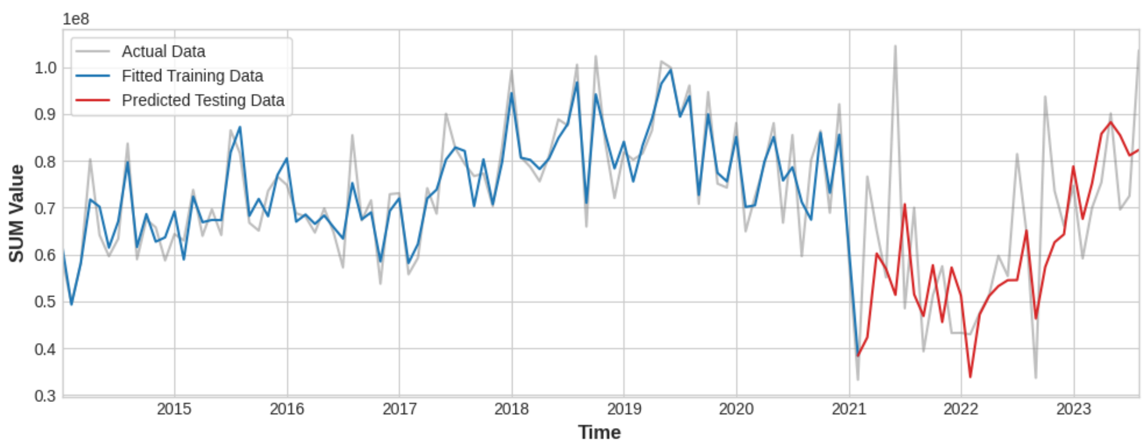


However, based on the output graph, the model failed to capture the downturn in the period around 2020 and the rebound after 2022. This trend is likely attributed by the impact of pandemic and its recovery phase, which also contributed to the fluctuations of carrier rates. Carrier rates are the fees that shippers pay to carriers for the transportation of goods from one location to another. One indicator that can reflect changes in carrier rates is the increasing percentage rate of Earnings Before Interest and Taxes (EBIT) among major ocean carriers (Ezinna et al., 2022). This reflects the profitability of ocean carriers due to elevated shipping costs paid by shippers. The changes in carrier rates can significantly affect the demand for shipping services, as shippers may alter their logistics mode based on the cost of transportation.

Therefore, we included the increasing percentage rate of EBIT of the main ocean carriers as an input feature to the second model being used for training the residuals, to help the model capture the downturn and rebound during the pandemic period. Due to the limited accessible open-source data regarding the increasing rate of EBIT of main ocean carriers, Figure 4-5 illustrates the performance of the updated model starting in 2014.

Figure 4-5

Boosted Hybrid Model with EBIT for Aggregated Value of Commodity Identified by HS Code 84 and 39



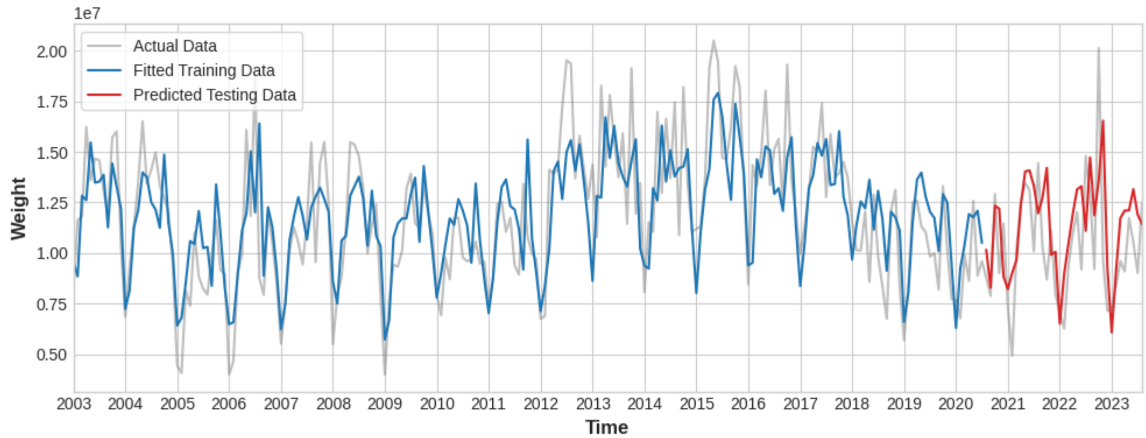
On the other hand, we also analyzed commodities with the highest weight: HS Code 22 Beverages, Spirits and Vinegar. With the same approach, liquids' weight showed a more stable trend and seasonality. Figure 4-6 shows the boosted hybrid model for the weight of beverages.

4.3.3 XGBoost

In order to fully harness all the time series features derived from the observed target dataset, considering the assumption of monthly seasonality throughout a year, we first constructed an initial set of features. This included lagged values ranging from 1 to 12 months and moving averages ranging from 2 to 12 months. An original

Figure 4-6

Boosted Hybrid Model for Weight of Commodity Identified by HS Code 22



XGBoost has been trained with both the initial set of values and additional time features, such as month, year, day of the week, and day of the month. To mitigate the risk of overfitting, we evaluated the importance of all the input features and identified the most influential lagged and moving average features. The model was then refined by retraining exclusively with these most influential features and fine-tuned by early stopping at the 50th round, thereby enhancing the model's robustness and generalization.

Figure 4-7 and Figure 4-8 present the performance of the XGBoost as applied to case studies concerning the aggregated value of commodities identified by HS Code 84 and 39 and the weight of commodities identified by HS Code 22, where the gray line represents the actual observed data, the blue line represents the fitted data on the training dataset, and the red line represents the predicted data on the testing dataset.

4.3.4 Error Measurements

As described in Section 3.6, error measurements MAE, RMSE and MAPE are applied to evaluate the performance of the above-mentioned models. Table 4.2 presents the results, where aggregated value represents the aggregated containerized value of commodities identified by HS Code 84 and 39, and weight represents the containerized

Figure 4-7

XGBoost Model for Aggregated Value of Commodity Identified by HS Code 84 and 39

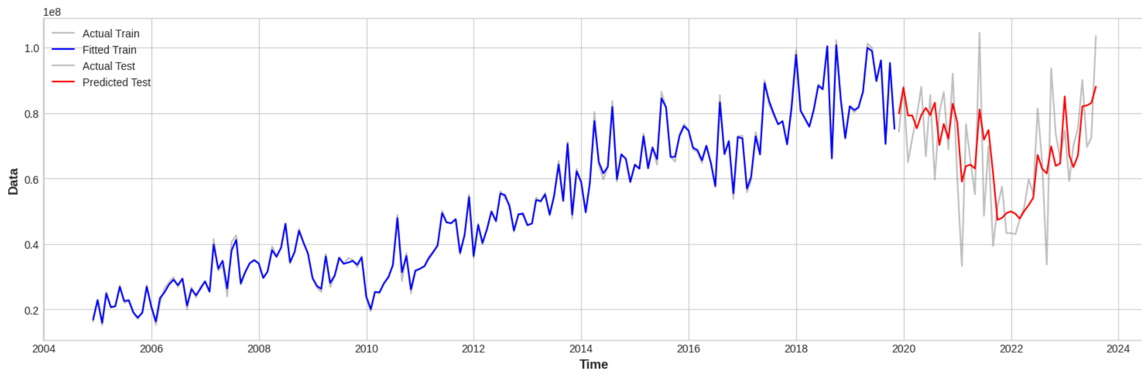
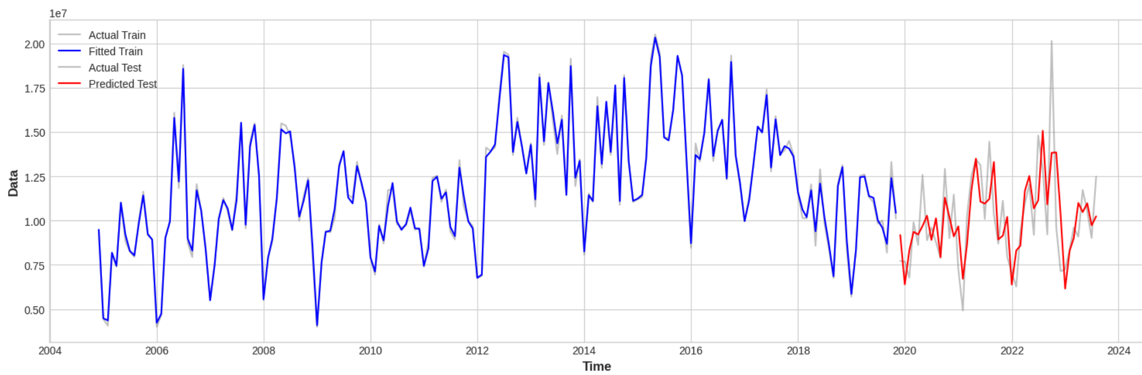


Figure 4-8

XGBoost Model for Weight of Commodity Identified by HS Code 22



weight of commodities identified by HS Code 22.

Table 4.2

Results of Error Measurements

	Aggregated Value			Weight		
Methods	MAE	RMSE	MAPE	MAE	RMSE	MAPE
Holt-Winters	20.74	26.18	36.78%	1.72	2.20	18.48%
Auto ARIMA	21.96	27.78	39.71%	3.90	4.24	44.48%
Boosted Hybrid	11.96	16.93	18.03%	2.17	2.73	22.87%
XGBoost	10.15	12.54	17.09%	1.62	2.02	16.33%

Note. The data presented in the MAE and RMSE columns are expressed in units of 10^6. Boosted Hybrid Model for aggregated containerized value is with the feature EBIT.

Chapter 5

Conclusion

In this chapter, we summarize the key findings from our research on the congestion of ports and imported flow of commodities. We also propose recommendations for future research or practical applications.

5.1 Congestion Points

DBSCAN showed good results in the initial determining areas of our models. However, it is possible to take further steps to automate terminals' and waiting areas' precise detection. This could also help with historical changes of the zones and automatic calculations of metrics, especially with all ongoing infrastructure projects for increasing the capacity of the ports.

5.2 Prediction Models for Congestion

To increase prediction capability, it would be helpful to incorporate additional data. First, it is necessary to have information about ships departing from the destination ports outside the USA, as this gives more precise information for the first port of entry. Also, missing information about the Panama Canal does not allow a correct diagnosis of goods flow disruptions. Additionally, research should be conducted to understand why models perform differently across various terminals in the system -

some models excel with certain terminals while performing poorly with others.

Another improvement may lie in knowing data about port operations, such as port yard utilization and the ability to serve ships quickly. This information could be obtained directly from the ports or could be received indirectly by other means.

Another valuable approach for stakeholders would be to utilize dynamic graph neural networks to predict potential ship diversion and changes in routes. There are several works addressing changes in graphs, for example, Z. Zhang et al. (2022) or Li et al. (2023)

5.3 Prediction Models for Commodities

In this study, we proposed different statistical and machine learning models to address the prediction problem of commodities' containerized value and weight. We applied Holt-Winters, ARIMA, boosted hybrid and XGBoost models to capture the trend and seasonality in the historical observed datasets.

5.3.1 Conclusion

According to the error measurements, XGBoost presented the best performance compared to other methodologies, with the least MAE, RMSE and MAPE. In our approach to building the XGBoost model, we intentionally selected the most influential features among lagged values and simple moving averages. However, as shown in the fitted data on the training dataset in Figure 4-7 and Figure 4-8, there is a great possibility of overfitting.

In summary, the input features utilized in the applied models in this study were mostly derived from historical observations. This indicates that the above-mentioned models are robust and general enough to apply across various ports and commodities. As stated in Section 2.2, the capability to predict the containerized value and weight of incoming commodities with relative precision enables port authorities to allocate human resources, crane utilization and warehouse capacity more effectively.

5.3.2 Future Research

As discussed in Section 5.3, there is a need to refine the input features used in the XGBoost model to improve its reliability. Although the current model included only the most important features ranked from lagged data and moving averages, the fit to the training dataset still suggested overfitting. To address this, more fine-tuning methods could be tested to reduce overfitting.

On the other hand, the case of the boosted hybrid model of aggregated containerized value with and without EBIT indicated that more exogenous variables could be considered when training the non-linear model targeting the residuals derived from the linear model.

We plan to integrate the results of congestion points into the current models for commodities. This will help improve the accuracy of the prediction for the value and weight of incoming shipments, taking into account the potential congestion situation near the port or along the shipping routes.

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Appendix A

Tables

Table A.1

List of Ports in ST-GNN Model

Port	Terminal	Model Notation
New York / New Jersey	APM Terminals	NY_APM
New York / New Jersey	Maher Terminals	NY_Maher
New York / New Jersey	The Red Hook Container Terminal	NY_Redhook
New York / New Jersey	Port Newark Container Terminal	NY_Newark
New York / New Jersey	Port Liberty Bayonne Terminal	NY_LibertyBayonne
New York / New Jersey	Port Liberty New York Terminal	NY_LibertyNewYork
Boston	Conley Terminal	Boston_Terminal
Savannah	The Port of Savannah	Savannah_Terminal
Norfolk	Norfolk International Terminals	Norfolk_Terminal
Baltimore	The Seagirt Marine Terminal	Baltimore_Terminal

Table A.2

Errors by Terminals, Models

Port Terminal	Model	MAE	MAPE	SMAPE
The Seagirt Marine Terminal	LSTM	0.94	33.55	33.73
	STGNN	1.27	30.81	40.51
	XGBoost	**0.34**	**16.25**	**14.13**
Conley Terminal	LSTM	**0.81**	**48.48**	112.21
	STGNN	1.08	61.74	**105.13**
	XGBoost	0.81	55.55	110.25
Norfolk International Terminals	LSTM	1.36	39.97	42.15
	STGNN	1.27	48.41	39.27
	XGBoost	**0.43**	**14.03**	**13.17**
APM Terminals	LSTM	1.57	37.64	47.08
	STGNN	1.52	55.16	41.05
	XGBoost	**0.52**	**12.28**	**12.82**
Port Liberty Bayonne Terminal	LSTM	0.70	50.68	84.62
	STGNN	**0.51**	**37.75**	**45.18**
	XGBoost	0.67	58.92	54.50
Port Liberty New York Terminal	LSTM	**0.77**	69.084	149.64
	STGNN	1.18	69.53	120.01
	XGBoost	0.84	**58.44**	**116.91**
Maher Terminals	LSTM	1.57	39.42	36.33
	STGNN	2.35	34.28	45.64
	XGBoost	**0.78**	**16.57**	**17.48**
Port Newark Container Terminal	LSTM	1.52	37.00	54.60
	STGNN	3.98	52.36	74.45
	XGBoost	**0.39**	**9.47**	**15.98**
The Red Hook Container Terminal	LSTM	**0.36**	**57.94**	158.42
	STGNN	1.39	79.62	147.71
	XGBoost	0.94	72.32	**146.14**
The Port of Savannah	LSTM	3.20	33.70	43.31
	STGNN	**1.98**	26.35	24.37
	XGBoost	2.01	**21.25**	**24.06**

Note. In bold shown the best error per terminal