Research on the potential of machine learning in predicting the relative abundance of Vibrio spp. on microplastics

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Abstract: Microplastics are a persistent and widespread pollution existing in the environment. Despite recognizing the harmful effects of MPs on human health and the ecosystem, researchers have suggested that MPs can serve as vectors in spreading pathogens. This highlights the urgency of developing a machine learning model to assess the associative risks. After analysing the global wastewater treatment plant distribution and the corresponding waste discharged, we identified that Bohai Sea deserves significant attention due to its high level of pollution and potential risks for pathogen transmission via microplastics. As a result, in this study, we developed an Artificial Neural Network model to predict the relative abundance of Vibrio spp. on the surface of microplastics in the Bohai Sea, China. Specifically, 483 data points were utilized to train the model, which incorporates environmental parameters such as temperature, salinity, dissolved oxygen, pH, total nitrogen, and total phosphorus. With a determination coefficient (R^2) of 0.87 and a mean absolute error (MAE) of 5.8, our model indicates a moderate level of accuracy, with improved performance in predicting middle-ranged data compared to extreme data. In the future, we can use more comprehensive datasets to explore the role of microplastics in transmitting other pathogens and toxic substances, which will provide insights into preventing disease infections and reducing marine pollution.

1. Introduction

Microplastics (MPs) are commonly known as synthetic insoluble plastic particles that are smaller than 5 mm. They can be produced either through primary or secondary manufacturing, originating from plastic bottles, personal care products, fishing gear, and other goods [1]. Primary manufacturing occurs when the size of the produced plastic particles matches that of MPs. For example, during the pre-production process of plastic pellets, producing MPs is unavoidable when the raw material of plastic is manufactured. Then the produced MPs can be released into the surroundings when plastics are being made, packed, and transported. For secondary manufacturing, MPs, such as microplastic fibers from washing machines and tire wear, are produced during the breakdown of large-sized plastic materials [2]. Previous studies have shown that a combination of ultraviolet and mechanical abrasion factors produces 76.5% of undetectable MPs, constituting a large proportion of the initial expanded polystyrene [3]. To date, the number of MPs is still growing. It is estimated that MPs will rise from 0.8 million tons in 2019 to 1.1 million tons in 2060 worldwide [4]. These astonishing statistics highlight the importance of ongoing government regulations and microplastic management.

Due to the persistent nature of plastics and the increasing demand for plastic products, MPs are ubiquitous. Not only do MPs exist in urban areas but also in remote areas, such as the Mariana Trench [5, 35]. MPs are also accumulated on land, such as agricultural land and soil sediments [6-7], in water, including marine and freshwater environments [8], in air [9], and within the human body [21]. Recently, it has been reported that MPs are hazardous to the environment. For instance, MPs contamination changes the physicochemical properties of soil, leading to reduced soil fertility [7]. Du and Wang reported that MPs would lead to negative impacts on the growth of terrestrial plants and influence soil microbial activity, and then inevitably threaten the ecosystem [12]. Furthermore, due their large surface area and hydrophobic property, MPs can act as “magnets” absorbing and spreading toxic materials in marine environments [24, 30]. Aquatic species ingest MPs from wastewater

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emissions, and MPs then enter the food chain and the marine ecosystem, leading to adverse impacts on aquatic organisms' metabolism, fertility, and mobility [13].

Except for the detrimental environmental effects of MPs, the existence of MPs also poses potential threats to human health. There are two main pathways for MPs to enter the human body: consumption and inhalation. Previous studies have reported that MPs are found in seafood [34], drinking water, beverages [16], dairy products [17], tea [32-33], fruits, and vegetables [31]. Studies have demonstrated that an average of over 5,800 pieces of MPs is ingested by a person per year from tap water (88%), beer (9%), and salt (3%) [42]. MPs are also accumulated in the digestive tracts and gill tissues of fish samples [18]. It is reported that a maximum of 53,865 particles of MPs can be consumed by a human through seafood each year, indicating the severity of MPs ingestion through diet [28]. Additionally, about 526 small fragments or fiber-shaped MPs items are accumulated in human airways per day [11]. Exposure to MPs through inhalation is raising researchers' concerns. Furthermore, MPs in the human body will cause cellular damage and severe health issues. In the digestive system, MPs might change intestinal microbiota and cause toxicity, leading to gastrointestinal symptoms. MPs may also transport toxins into human airways and lungs, causing oxidative stress, respiratory symptoms, and an increased risk of pulmonary disease. Moreover, MPs, along with environmental toxins, may interfere with hormone receptors and mimic hormones, leading to endocrine disorders [10]. MPs are also discovered in the placentas of pregnant women, which suggests the potential negative impacts on their reproductive systems and the newborns [19-20]. Overall, a non-negligible number of MPs enters human bodies through consumption and inhalation, causing potential negative effects on the digestive, respiratory, immune, and reproductive systems [18].

Since MPs can cause harm to both the environment and human health, it is necessary to investigate their impact on the ecosystem. In this study, a comprehensive dataset with parameters including temperature, salinity, dissolved oxygen, pH, total nitrogen, total phosphorus, and relative abundance of Vibrio spp. on MPs was established. The Artificial Neural Network (ANN) was employed to predict the relative abundance of Vibrio spp. on MPs based on the dataset related to the Bohai Sea in China. The ANN model achieved a moderate level of performance with a determination coefficient (R^2) of 0.87 and a mean absolute error (MAE) of 5.8.

2. Problem Definition

Previous studies have shown that WWTPs are a dominating source of MP pollution in the marine environment, since approximately 1.4 billion particles are emitted into the ocean per day [22]. Therefore, understanding the distribution and severity of MP emission from WWTPs worldwide can provide critical insights into the treatment and targeted management of MPs pollution in the aqueous environment.

Figure 1A is a scatter plot presenting the distribution of global WWTPs using their coordinates and the magnitudes of wastewater discharged. Figure 1B exhibits the waste discharged volumes for each WWTP, where the bubble size is directly proportional to the waste discharged volume (106 m3 d-2). As seen in Figure 1A, a large number of WWTPs are concentrated in the United States and Europe. This may be ascribed to their early industrialization and well-established wastewater treatment facilities. Additionally, there is a significant number of WWTPs present in Asia, specifically in densely populated places such as southeast China, Japan, and India. This result indicates that there is an effort in managing and treating wastewater in populated locations, and the number of WWTPs might be positively correlated with population density. However, most of the WWTPs in Africa are located in the southern part, with a negligible number in the northern part. This might be due to the lack of installation of WWTPs in the northern part of Africa. Additionally, the distribution of WWTPs in South America and Australia is mostly along the east and west coasts, which is similar to the distribution of populations [26].

Moreover, Figure 1B takes into account the magnitude of hydro waste discharged by WWTPs. It shows that large bubbles dominate the United States and east China, indicating high levels of waste discharged by WWTPs in these areas. This aligns with the observations from Figure 1A. In addition, although there are numerous data points plotted in Europe and Japan in Figure 1A, their bubble sizes in Figure 1B are relatively small. This implies that despite the large number of WWTPs present in Europe and Japan, their individual waste treatment capacities are smaller than those in the United States and East China. Furthermore, the bubbles in South America, Africa, and Australia are minimal in magnitude; this may be due to lower population densities in these areas compared with the United States and East China. Comparing Figure 1A and Figure 1B, we can infer that the number of WWTPs present does not necessarily correlate with the amount of hydro waste emitted. Moreover, the magnitude of waste discharged can potentially reflect the population density and the degree of industrialization in these areas. These relationships can provide insights into wastewater management and global water environment protection.

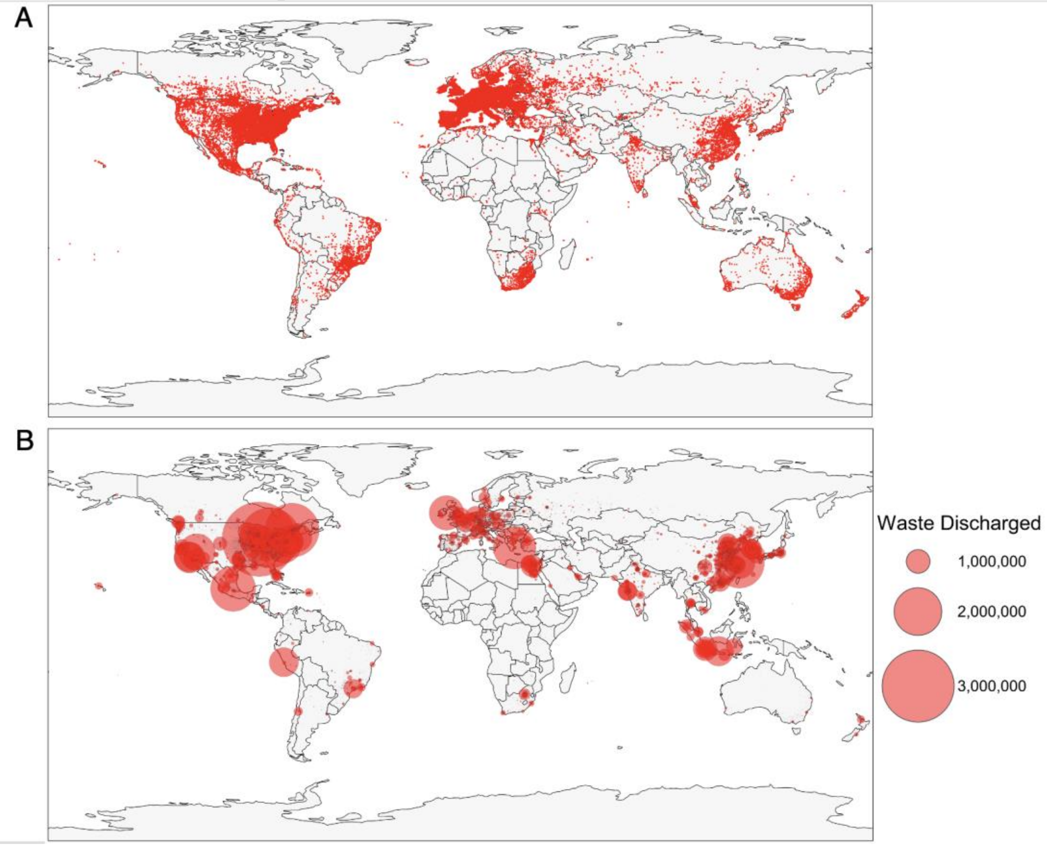

Figure 1. Wastewater treatment plant (WWTP) distribution and waste discharged around the world.

Recently, there has been a growing consensus among researchers that MPs can act as vectors for transporting hazardous substances. It has been reported that large populations of bacteria from distinct communities are attached to plastic surfaces [29]. Due to anthropogenic and environmental factors, MPs contamination is distributed across the world. A previous study has shown that bacterial pathogens and algae can be transmitted in ballast water via MPs [27]. With an increasing number of MPs existing in the ocean, along with an abundance of harmful pathogens being transmitted, potential disease outbreaks and harmful algal blooms might occur.

Vibrio, belonging to the class Gammaproteo-bacteria, is a type of waterborne detrimental pathogen. Vibrio can cause human infections through the ingestion of contaminated seafood and water [25]. A previous study has shown that the Vibrio species causes almost 50% of the foodborne outbreaks in Asia [39]. Over the last 15 years, there has been an increasing trend in the number of Vibrio infections in the United States [14]. Recently, researchers have found that Vibrio can be widely spread across the world. For example, Vibrio species are detected on MPs in the North and Baltic Sea water samples [15]. As a result, there is an urgent need for a more comprehensive understanding of the association between MPs and Vibrio spp. In this study, we collected data on MPs and the physicochemical parameters of the water body from the Bohai Sea in China. Using this data, we developed a machine learning model with ANN to predict the relative abundance of Vibrio spp. in the biofilms on the surface of MPs in the Bohai Sea.

3. Related Research

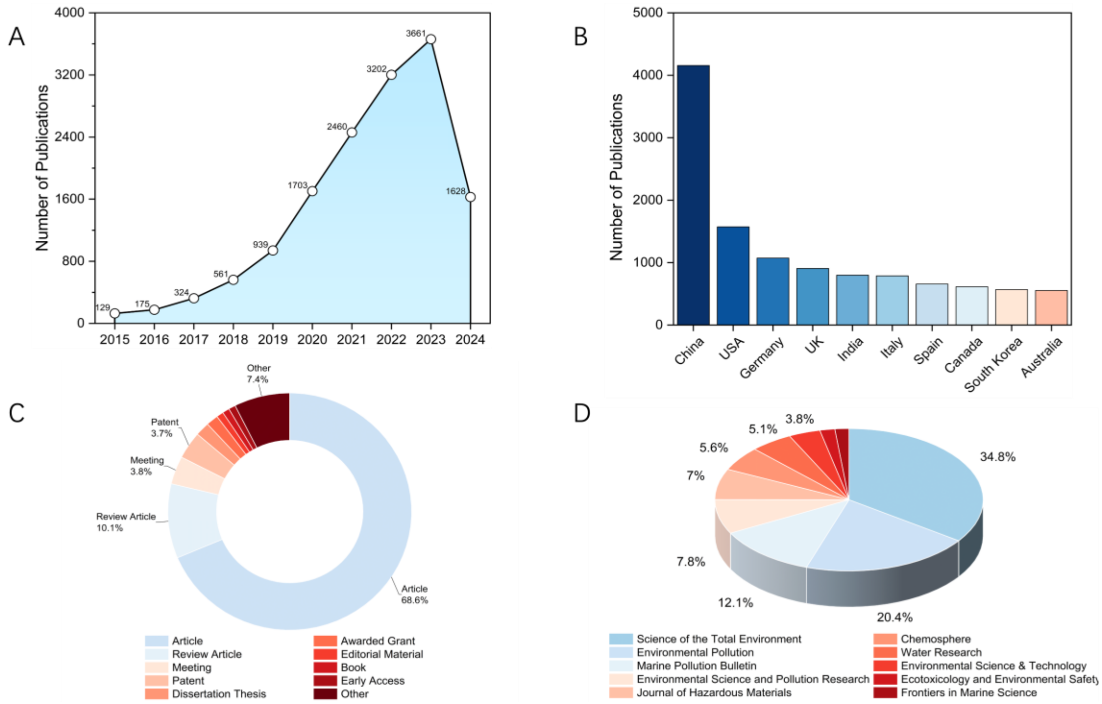

Figure 2. Statistics on the number of publications related to MPs on Web of Science database.

In this section, we investigated the research trends in MPs from 2015 to 2024 using a bibliometric analysis method on the Web of Science database, a comprehensive database containing scholarly literature and citations across multiple fields of disciplines. We searched for "Highly Cited Papers" and "Hot Papers," excluding "Review Articles" and "Open Access," related to MPs. The statistical analysis of the searched publications was performed using Python programming language version 3.10.12.

Figure 2 presents the analysis results of the publications. Figure 2A shows the trend in the number of publications on MPs from 2015 to 2024. Figure 2B presents the top 10 countries by the number of MPs research publications. Figure 2C highlights the top 10 document types by the number of MPs research publications. Figure 2D displays the top 10 journals by the number of MPs research publications. As seen in Figure 2A, there was an increasing trend in the number of publications from 2015 (129 papers) to 2023 (3661 papers). The number of published articles in 2023 was 14 times that of 2015. The result indicated that MPs issue was attracting concerns from researchers. As shown in Figure 2B, China occupied the largest number of published papers related to MPs, followed by the United States, Germany, the United Kingdom, India, Italy, Spain, Canada, South Korea, and Australia. In this period, more than 4000 papers were published by China from 2015-2024, which was over twice the number published by the United States and many times more than other countries. Furthermore, according to Figure 2C, articles were the most prevalent document type, with between 12000 and 14000 publications, which was significantly higher than other document types. Moreover, as illustrated in Figure 2D, most of the publications were published in the journal "Science of the Total Environment," followed by "Environmental Pollution," "Marine Pollution Bulletin," "Environmental Science and Pollution Research," "Journal of Hazardous Materials," "Chemosphere," "Water Research," "Environmental Science & Technology," "Ecotoxicology and Environmental Safety," and "Frontiers in Marine Science."

Moreover, the searched publications from Web of Science were analyzed using VOSviewer (version 1.6.20).

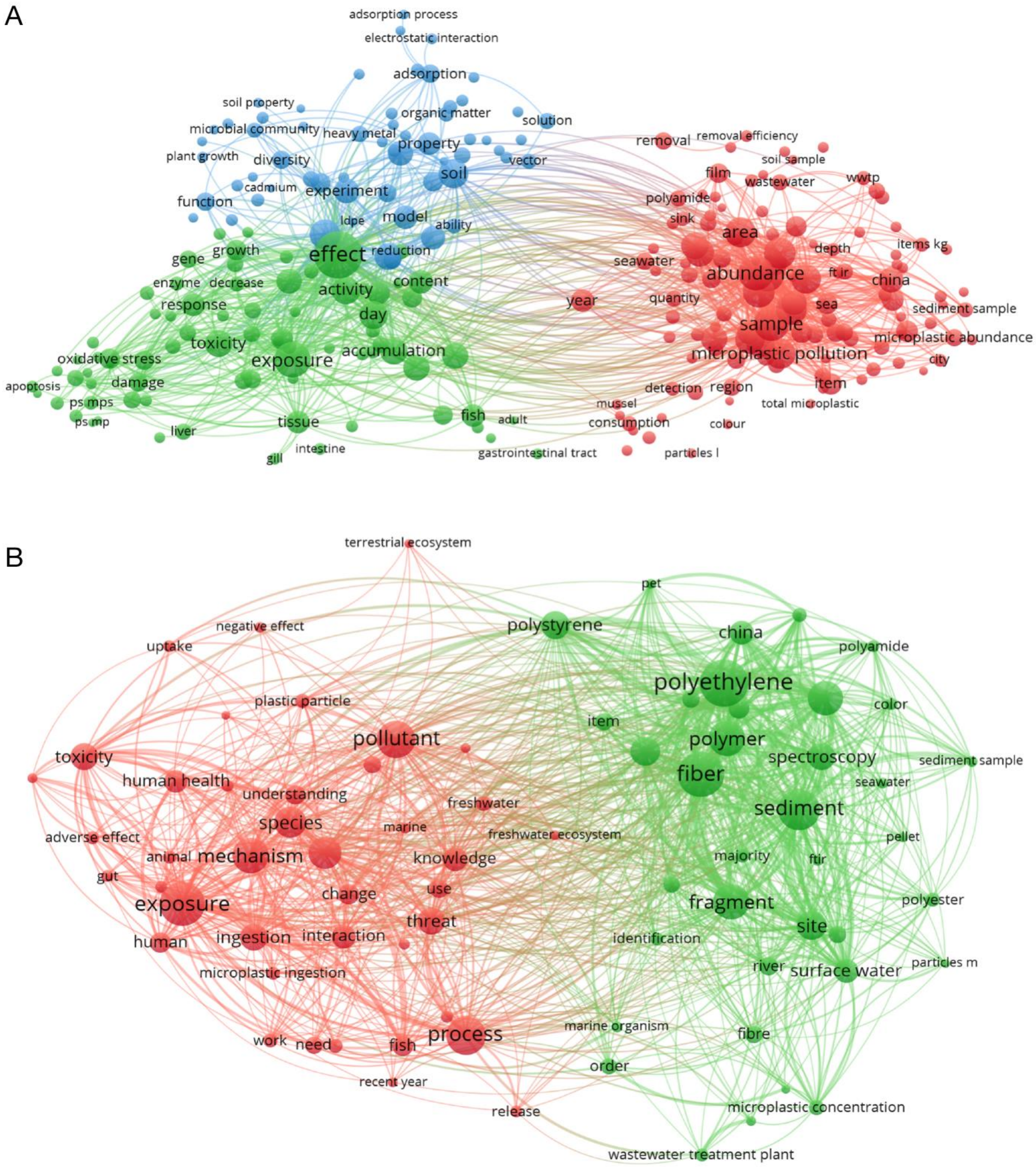

Figure 3. VOSviewer visualization of keywords used in papers relating to MPs.

The software VOSviewer (version 1.6.20) is a powerful tool to analyze the co-occurrence networks of key terms from academic papers [38,41]. It can provide an overview of the main research topics in the scientific discipline as well as the correlations between topics. The keyword “microplastics” was chosen to search for publications from the Web of Science. We plotted two figures: Figure 3A is a VOSviewer visualization of publications related to MPs, and Figure 3B is a VOSviewer visualization of "highly cited papers" and "hot papers" related to MPs. As shown in Figure 3, VOSviewer was used to analyze, cluster, and map data from the collected articles. The diameter of each circle is determined by its assigned weight. A big circle represents a high value of weight, and vice versa.

First, we took an overview of the existing articles related to MPs. We selected 816 articles from the Web of Science database and extracted the terms occurring with VOSviewer. The filtration criteria stipulated that a term should appear no less than 12 times. Among the 17,228 terms, 425 of them satisfied this requirement. The 60% most relevant terms were selected based on their calculated relevance scores. After manually deleting irrelevant terms, 248 terms were mapped and visualized in Figure 3A. The terms were categorized into three groups, with 118 terms presented in the red cluster, 78 terms presented in the green cluster, and 59 terms presented in the blue cluster. Table 1 shows the top 30 most common terms, along with their respective weights of occurrences and total link strength.

Table 1: Top 30 most frequent words appear in publications related to MPs.

Keyword	Weight of occurrences	Weight of total link strength
exposure	184	2267
abundance	176	2457
sample	173	2191
source	150	1819
polypropylene	149	2011
distribution	141	1927
microplastic pollution	139	1882
area	139	1789
fiber	133	1802
mechanism	132	1661
soil	128	1642
fragment	127	1729
sediment	126	1688
activity	118	1670
polymer	115	1461
shape	113	1563
characteristic	112	1496
accumulation	109	1429
toxicity	108	1403
occurrence	103	1380
pathway	103	1380
health	100	1164
interaction	96	1138
site	93	1286
change	91	1187
china	90	1338
experiment	89	1011
model	88	1038
treatment	83	1099
spectroscopy	79	1094

The red bubble cluster indicated sampling, geographical location, and experiment methodologies in MPs papers. Keywords such as “soil sample,” “seawater,” “wastewater,” and “sediment sample” showed that various studies included sampling MPs from different types of sources. Keywords like “area,” “city,” “WWTP,” and “China” suggested that multiple investigations were dedicated to understanding the sites and geographical spread of MPs. From the bubble “FTIR” (Fourier-transform infrared spectroscopy), we inferred that this detection method was often used in the experiments on MPs.

The green bubble cluster contained words associated with biological impact and toxicity. Keywords like “tissue,” “liver,” “intestine,” “gill,” and “gastrointestinal tract” implied that studies focused on the biological effects of MPs on tissues and organs. Keywords like “oxidative stress” and “apoptosis” indicated studies of the influence of MPs on biological responses. Keywords such as “genes” and “enzymes” suggested research focusing on the effect of MPs on the basic mechanisms of organisms. Keywords like “toxicity” and “damage” presented research that involved examinations of the overall harmful effects of MPs.

The blue bubble cluster focused more on the interaction between MPs and soil. Studies explored the effect of MPs on “soil property,” “microbial community,” and “plant growth.” They also included the role of MPs in the absorption process, such as the absorption of heavy metals. Besides, investigations also concentrated on the chemical processes of the interaction between MPs and other environmental components, which was evident in the keywords “electrostatic interaction” and "organic matter."

Additionally, we were curious about the most popular topics related to MPs investigated by scholars in recent years, which provide insight into the world's leading concerns regarding MPs. Extracted from the Web of Science database, 290 research articles published between 2014 and 2024 from the "highly cited papers" and "hot papers" categories were selected. Examined using VOSviewer, 140 of the 7,214 terms met the criteria of occurring at least 12 times. Based on the calculated relevance score for each term, the 60% most relevant terms were selected and screened for visualization. The data were grouped into two categories by cluster analysis, with 41 terms in the first group and 37 terms in the second group. After manually removing several non-pertinent terms, the top 30 most frequently appearing terms along with the number of occurrences and the total link strength are displayed in Table 2.

Table 2: Top 30 most frequent words appear in "highly cited papers" and "hot papers" related to MPs

Keyword	Weight of occurrences	Weight of total link strength
polyethylene	61	536
fiber	58	425
exposure	57	374
sediment	52	411
process	49	292
pollutant	48	313
polymer	46	368
fragment	45	370
mechanism	45	260
polypropylene	44	419
accumulation	41	271
species	40	276
composition	38	320
site	38	311
polystyrene	36	304
threat	35	258
ingestion	35	243
toxicity	35	210
spectroscopy	34	307
surface water	31	275
china	31	263
knowledge	30	228
interaction	30	171
human health	29	183
change	27	174
polymer type	26	226
fish	26	199
human	26	184
understanding	25	164
river	24	193

The red cluster concentrates on the adverse effects and toxicity of MPs. For instance, Wang et al. discussed the potential hazard of MPs to humans, and found that particles can pass across the respiratory barrier and accumulate in people's secondary organs [40, 48]. In addition, the author also reported the physical and chemical impacts of MPs on marine biota and freshwater biota. Decreased lipid stores, ulcers, and toxicity of absorbed contaminants can be induced, leading to harmful effects on the health of different organisms. A previous study also presented the concentration, spatial distribution, and the possible mechanism of the absorption and desorption of toxic contaminants from MPs [47]. Furthermore, Ren et al. [46] investigated the co-occurrence relationship between microplastics and microcystins in marine environments, then highlighted that MPs could serve as a medium to transport microcystins, which led to a higher level of accumulation in marine animals.

The green cluster focuses on the classified types, chemical components, and sources of MPs. According to an existing study, polypropylene, polyethylene terephthalate, polyethylene, polyurethane, polystyrene, and polyvinyl chloride are the dominant chemical components of MPs [45]. Besides, due to the physical and chemical properties of these components, He et al. illustrated that the biofilms grown on MPs exhibited slightly different characteristics and performances in terms of microbial adhesion and bacterial abundance [44]. For instance, compared to polypropylene, polyvinyl chloride had better microbial adhesion due to its weaker bond strength and increased surface area. Moreover, scholars have conducted numerous studies on terrestrial and ocean sources of MPs. Duis and Coors. [43] reported that approximately 80-90% of MPs come from land-based sources, which is significantly higher than the number of MPs originating from ocean-based sources.

4. Methodology and Description of Key Components

A total of 483 data points were collected from Jiang's publication, with 315 data points measured from the Sungo Bay mariculture zone and 168 data points measured from the Haihe Estuary [36]. The physicochemical parameters of sea water (temperature, salinity, dissolved oxygen, pH, total nitrogen, total phosphorus) and the relative abundance of Vibrio spp. were included in the dataset [37].

Machine learning models, such as random forest, generative adversarial networks, deep neural networks, and ANN, are popular used to solve environmental issues in recent years [23]. Among these models, ANN is reported to be widely utilized in water quality and pollution research [12]. In this study, ANN was selected to predict the relative abundance of Vibrio spp. based on the collected parameters. The R^2 and MAE were calculated to evaluate the model performance according to (1) and (2).

$$R^2 = 1 - \frac{\sum_{i=1}^{m}(X_i - \mathrm{Y}_i)^2}{\sum_{i=1}^{m}(\bar{Y} - \mathrm{Y}_i)^2} \tag{1}$$

Where X_i is the predicted value with index i, Y_i is the true value with index i, $\bar{Y}$ is the mean of the actual values and m is the number of values.

$$\mathrm{MAE} = \frac{\sum_{i=1}^{m}|X_i - Y_i|}{m} \tag{2}$$

Where X_i is the predicted value with index i, Y_i is the true value with index i and m is the number of values.

5. Experiment

Figure 4 shows the dynamic workflow of this experiment. After inputting the environmental parameters, the data was first normalized to a scale ranging from 0 to 1 based on z-score method calculated according to (3). Data normalization can significantly speed up the calculation process, yield better results, and ensure certain parameters do not overly influence the outcome of the machine learning model. Then, the data were randomly split into the training and testing datasets. As a result, 87% of the total data were labeled as training data and the remaining 13% of the total data were labeled as testing data. Finally, model prediction performance was evaluated with calculated R^2 and MAE.

$$z = \frac{\chi - \mu}{\sigma} \tag{3}$$

Where χ is the observed value, μ is the average value of the sample, and σ is the standard deviation of the sample.

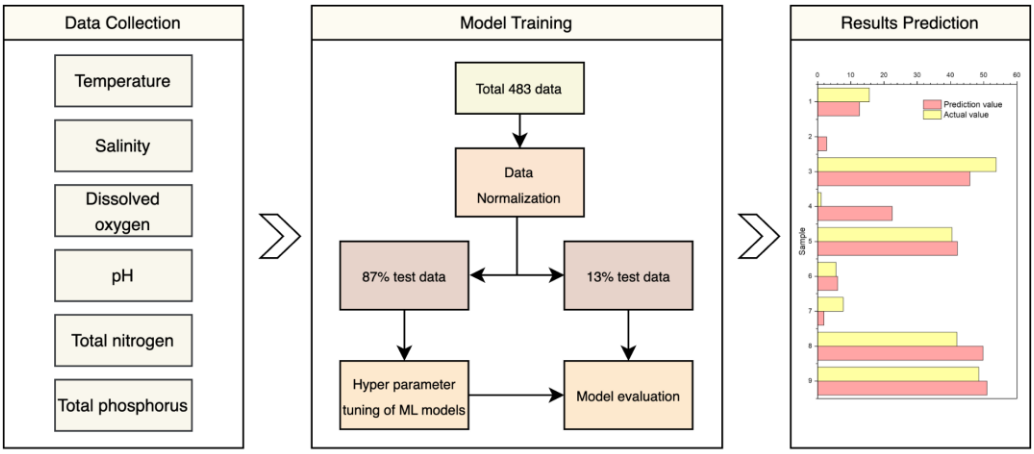

Figure 4. Schematic flowchart for predicting the relative abundance of Vibrio spp.

6. Data Analysis

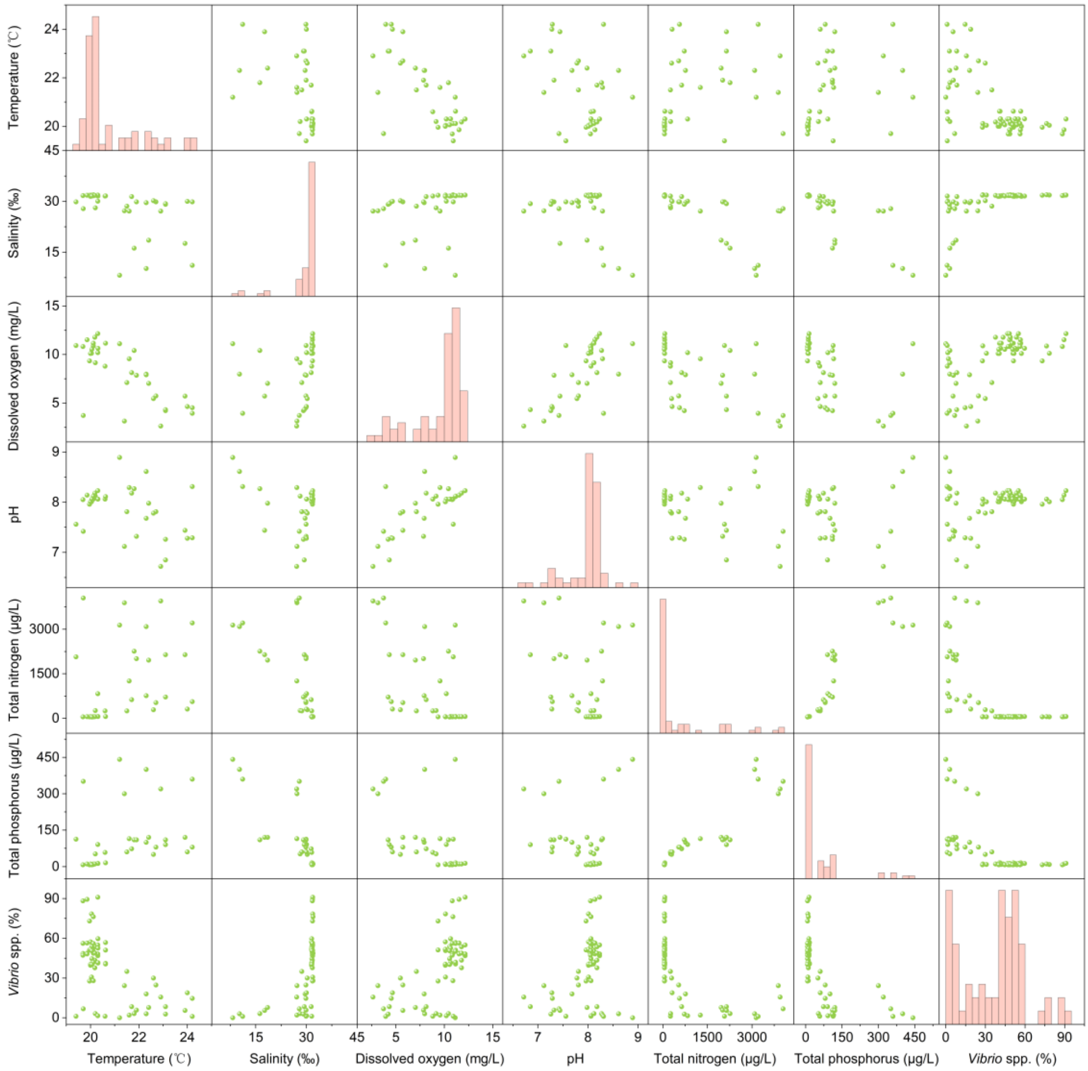

Figure 5. Scatter matrix for collected parameters

According to Figure 5, the temperature ranged from 19.4℃ to 24.2℃, with a concentration around 20.1℃. The dominant value of salinity was around 30‰, with a maximum value of 31.95‰ and a minimum value of 8.21‰. Dissolved oxygen varied between 2.64 mg/L to 12.15 mg/L and was clustered around 11 mg/L. pH fluctuated between 6.72 to 8.89 and was centered around 8.1. Total nitrogen fell within the range of 47.08 μg/L to 4050 μg/L, with a predominant value around 10.0 μg/L. Total phosphorus was distributed between 7.42 μg/L to 442 μg/L and was concentrated around 10 μg/L. The relative abundance of Vibrio spp. ranged from 0 to 90.98%, focusing mainly around 10%, 5%, and 50%. Among the data, we noticed that the correlations between these parameters were non-linear, making it difficult to process the data using simple linear regressions. As a result, we applied a machine learning model algorithm, ANN, to process the data.

7. Performance Analysis

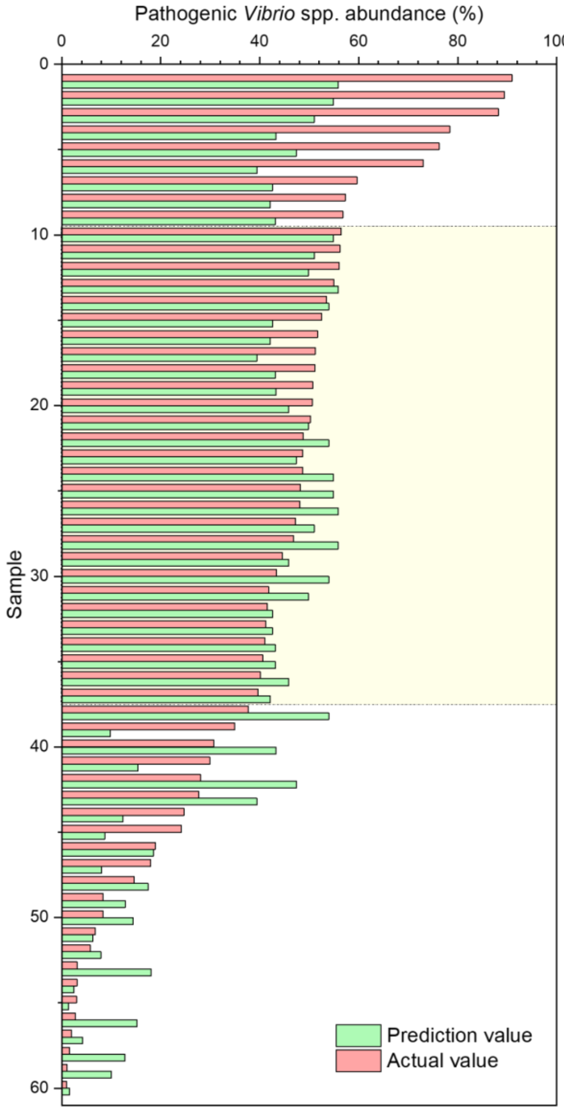

Figure 6. Comparisons between the real and predicted relative abundance of Vibrio spp. using ANN.

We tuned hyperparameters to achieve optimal performance for the ANN model. Figure 6 was generated using both the predicted values and the actual values from the training dataset. The R^2 for the training dataset was 0.87, and the MAE was 5.8. Additionally, we plotted Figure 6 using predicted values and actual values from the testing dataset, which contained 60 data points. The green bars represent the predicted values, while the red bars represent the actual values. For each sample, the more consistent the lengths of the green and red bars are, the better the prediction accuracy for that sample. If the green bar is longer than the red bar, then the data is overestimated, and vice versa. As observed in Figure 6, the ANN model exhibited good performance when the actual value of the relative abundance of Vibrio spp. lay within the middle range. This can be seen from the small discrepancy between the lengths of the green and red bars when predicting moderate levels of the relative abundance of Vibrio spp. In contrast, in the upper and lower parts of Figure 6, where the predicted values were more extreme, large prediction errors appeared. This indicated that the ANN model was more accurate in predicting middle-range relative abundance of Vibrio spp.

8. Overall Conclusion and Future Works

In this study, we utilized 483 data points with parameters including temperature, salinity, dissolved oxygen, pH, total nitrogen, total phosphorus, and the relative abundance of Vibrio species to build a dataset. Then, the ANN model was employed to predict the relative abundance of Vibrio species present on the surface of MPs. Our model achieved a moderate level of accuracy, with an R^2 of 0.87 and an MAE of 5.8. It performed better with middle-ranged data compared to extreme data.

Moreover, given the extensive scientific research on MPs, additional work is necessary. In the future, with a more comprehensive environmental parameter dataset, we can train more machine learning models to predict different pathogens from various oceans and continents. Additionally, research is required to further explore other potential substances, apart from pathogens, attached to MP surfaces in the aquatic environment, as well as their potential negative impacts on human health and marine ecosystems.

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