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Refining Marine Net Primary Production Estimates: Advanced Uncertainty Quantification through Probability Prediction Models

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Abstract

In marine ecosystems, Net Primary Production (NPP) is pivotal, not merely as a critical indicator of ecosystem health, but also as an integral component in the global carbon cycling process. This study introduces an advanced probability prediction model to refine the precision of NPP estimation and to deepen our comprehension of its inherent uncertainties. A comprehensive comparative analysis is undertaken, juxtaposing a Bayesian probability prediction model, predicated on empirical distribution, with a probability prediction model anchored in deep learning. The objective is to meticulously quantify the uncertainty associated with NPP. The findings underscore the applicability of probability prediction in investigating the uncertainty of marine NPP. Both models proficiently delineate the dynamic trends and inherent uncertainties in NPP, with the neural network model exhibiting superior

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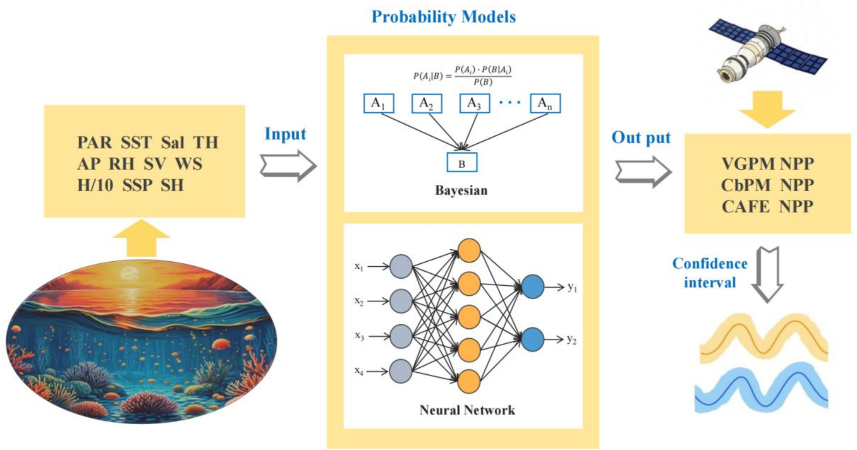
accuracy and dependability. Additionally, these probability prediction models are adeptly applied to prognosticate NPP in specific marine regions, efficaciously elucidating the interannual trends in NPP variation. This research contributes not only a more precise method for quantifying NPP uncertainty but also bolsters scientific support for the stewardship of marine ecosystems and the preservation of environmental integrity.

Keywords: Net Primary Production; Bayesian Probability Prediction; Neural Network Probability Prediction.



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1. Introduction

Net Primary Production (NPP) of phytoplankton, an indispensable indicator for biological productivity, exerts a substantial influence on global carbon flux and the dynamics of marine ecosystems (Yang et al., 2021; Silsbe et al., 2016). The precision in estimating NPP is paramount for environmental quality assessments (Falkowski et al., 1998; Tan et al., 2005), effective fisheries resource management, and comprehending the impacts of global climate change (Lee et al., 2015; Ding et al., 2016). Conventional methods of NPP measurement, such as ship-based sampling and

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bottle incubations, are beset with challenges like human errors and inadequacies in capturing spatial and temporal dynamics. This underscores the necessity for more sophisticated and comprehensive methods (Yang et al., 2021; Li et al., 2020).

The advent of ocean observation satellites and ocean color remote sensing technology has catalyzed a paradigm shift in the estimation of large-scale marine primary productivity (Yang et al., 2021; Westberry et al., 2008). These pioneering technological advancements furnish novel insights into phytoplankton photosynthetic production and its integral role in the carbon cycle, thereby broadening the observational spectrum and establishing a robust foundation for predicting marine NPP. Initial remote sensing endeavors to estimate NPP, employing satellite-based chlorophyll-a (Chl-a) (Platt et al., 1991; Platt & Sathyendranath, 1988; Sathyendranath et al., 1995), stemmed from the established correlation between chlorophyll and photosynthesis (Ryther, 1956; Ryther & Yentsch, 1957). However, these efforts were predominantly confined to local or regional applications. A subsequent investigation by Campbell et al. (2002) delved into the accuracy of various satellite primary productivity algorithms, unveiling that estimates from the most effective algorithm often diverged from those derived from those obtained using the ^{14}C isotope labeling method. Their study also unearthed systematic biases in several algorithms, which could be alleviated through re-parameterization.

In response to the aforementioned limitations, several remote sensing-based models, such as the Vertically Generalized Production Model (VGPM), the Carbon-based Productivity Model (CbPM), and the Carbon, Absorption, and Fluorescence Euphotic-resolving model (CAFE), have been innovatively proposed (Behrenfeld et al., 1997; Westberry et al., 2008; Silsbe et al., 2016). Spanning various decades, these models address diverse facets of ocean primary production and are readily accessible via satellite remote sensing data platforms. As a result, they have been extensively applied and discussed in numerous studies (Westberry et al., 2008; Pan et al., 2012; Dave et al., 2013; Li et al., 2020; Yang, 2021; Cael, 2021).

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Particularly, VGPM formulates a light-dependent, depth-integrated model that classifies environmental factors influencing the vertical distribution and optimal assimilation efficiency of primary production, leveraging ^{14}C productivity measurement data (Behrenfeld et al., 1997). Conversely, CbPM was a depth-resolved spectral NPP model designed for phytoplankton growth rates (Westberry et al., 2008). Its foundational concept was originally articulated by Behrenfeld et al. (2005). Distinguishing itself from Chl-based models, CbPM enables the differentiation of physiological changes in biomass and Chl, thus offering a more nuanced depiction of phytoplankton production. Notably, its strength lies in addressing issues related to light and nutrient adaptation, thereby enhancing its capability in estimating fixed carbon output at the ocean surface. Similarly, the CAFE model, introduced in 2016, presents an adaptive framework that melds satellite ocean color analysis with essential physiological and ecological attributes of phytoplankton (Silsbe et al., 2016). It incorporates intrinsic optical properties into the model and calculates NPP by assessing the product of energy absorption and the efficiency of converting absorbed energy into carbon biomass, alongside computing growth rates. Nonetheless, these models commonly generate a single value of NPP, overlooking the range estimation and the inherent uncertainties in NPP estimation, stemming either from the model itself (BIPM et al., 2009) or from the model input (Milutinovic & Bertino, 2011). This oversight is critical, as suggested by Saba et al. (2011), since uncertainties in input variables, like Chl-a, significantly impinge upon model performance and accuracy. In a recent assessment, Westberry et al. (2023) examined the daily depth-integrated NPP rates over 2003–2018 for VGPM, CbPM, and CAFE, revealing that the mean NPP fields of CbPM and CAFE, along with their associated frequency distributions, are distinctly divergent from those of VGPM.

Transitioning from the constraints of traditional models, probabilistic forecasting, in contrast to deterministic forecasting (Juban et al., 2007), generates a cumulative distribution function or probability density function for the predicted object. This methodology offers a more holistic understanding of likely outcomes (Gneiting &

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Katzfuss, 2014; Schepen et al., 2018; Zhao et al., 2015). Significantly, this approach has been successfully implemented in fields such as hydrology (Schepen et al., 2018; Zhao et al., 2015; Schwanenberg et al., 2015) and power system management (Al-Gabalawy et al., 2021). For instance, Schwanenberg et al. (2015) conducted analyses using both deterministic and probabilistic forecasts. They concluded that deterministic forecasts tend to overlook forecast uncertainty in short-term decisions, whereas probabilistic forecasting offers numerous advantages: (i) it enables a longer forecast horizon, facilitating earlier and more accurate predictions of major events; (ii) stochastic optimization yields more robust decisions compared to deterministic procedures that focus solely on individual future trajectories; and (iii) it permits introduction of advanced chance constraints for refining the system operation.

Although Bayesian models and probabilistic neural networks are established methods, their application to the remote sensing of marine net primary productivity (NPP) represents a novel approach. This study leverages these advanced probabilistic techniques to address the unique challenges in estimating NPP from satellite data, providing a more accurate and reliable quantification of uncertainties. We introduce probabilistic prediction models to meticulously quantify the uncertainty of NPP estimation, thereby enhancing our comprehension of NPP's significance in marine ecosystems. The research objectives of this paper are articulated as follows: (1) to thoroughly quantify the uncertainty of NPP estimation through the integration of probabilistic forecasting; (2) To evaluate and contrast the efficacy of neural network-based probabilistic forecasting with empirical distribution-based Bayesian probabilistic forecasting in capturing NPP uncertainty; and (3) To implement probabilistic forecasting of the uncertainty of the NPP in the study area during 2007–2018 and to explore its temporal characteristics. Our study offers innovative perspectives and methodologies for addressing the uncertainty associated with NPP. The organization of this paper is as follows: Section 2 outlines the study area and data sources; Section 3 elaborates on the methodology and presents metrics for evaluating forecasting performance; Section 4 discloses the results; and Section 5 presents the

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conclusions.

2. Data and Methods

2.1. Study Area and Data Sources

The research locale for this study is situated in the aquatic environs of Weizhou Island, nestled within the Gulf of Tonkin, Guangxi Province, southern China (Fig. 1). The proportion of excellent water quality in Guangxi's near-shore waters reaches more than 90% all year round, and the quality of the marine ecological environment has remained at the forefront of the country for 12 consecutive years, which is the only stable habitat and feeding ground for large cetaceans known in China's near-shore waters at present. Weizhou Island is the youngest volcanic island in China geologically, with more than 95% of its strata comprising volcanic rocks, and landscapes of sea erosion, sea accumulation, and dissolved rocks. Surrounded by the sea on all sides, Weizhou Island is in the southern subtropical monsoon zone, with a pleasant climate, rich heat, and abundant precipitation throughout the year. The average annual temperature is 23℃, and the average winter temperature is 16.3℃. The unique climatic conditions and island landscape make it a popular tourist destination. The waters of Weizhou Island are the habitat of many rare marine organisms, and the protection and research of its marine ecosystem are of great significance to maintaining marine biodiversity.

The dataset of this study encompasses eight distinct sets of monitoring data spanning from January 2007 to February 2018, amassing a total of 4077 days. These data were procured from the Weizhou Marine Environmental Monitoring Station (21.0017°N, 109.0117°E) and encompass a spectrum of variables: sea surface temperature (SST), salinity (Sal), tide height (TH), air pressure (AP), relative humidity (RH), sea visibility (SV), wind speed (WS), and 1/10th significant wave height (H/10). Additionally, photosynthetically active radiation (PAR) was retrieved from NASA’s Ocean Color portal (https://oceancolor.gsfc.nasa.gov/), sea surface precipitation (SSP) was sourced from Nasa Earth Observation Data

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(https://www.earthdata.nasa.gov/), and sunshine hours (SH) was sourced from the China Meteorological Administration (https://data.cma.cn/). This compilation resulted in a comprehensive dataset comprising eleven variables. For the analysis of three NPP algorithms — namely, VGPM, CbPM, and CAFE — we acquired datasets at an eight-day temporal resolution from the Ocean Productivity website (http://orca.science.oregonstate.edu/npp.visual.php). This data acquisition process spanned a cumulative duration of 514 days. The specific datasets utilized for this study are itemized in Table 1.

Due to factors such as equipment malfunctions and adverse weather conditions, some data for the eleven variables were incomplete. To gain a deeper understanding of the data structure and address these gaps, we conducted an analysis of the missing data and identified five variables with missing entries (Table 2): SV, H/10, SSP, PAR, and SH. Subsequently, we visualized these five variables in a chronological sequence, with the findings depicted in Fig. 2. Distinct from daylength, which is computable based on location and date, SH indeed refers to the daily measured duration of sunlight reaching the Earth's surface. The variability and instances of zero values observed in Fig. 2 (bottom panel) and mentioned in Table 2 reflect real-world fluctuations due to weather conditions—on overcast or rainy days, actual sunshine hours recorded can indeed drop to zero. These data are collected on a daily basis, hence the seemingly sporadic pattern rather than a smooth temporal variation expected of constant daylength calculations. The analysis revealed a marked periodicity in these variables, prompting us to employ time series interpolation as our method of choice for data imputation. The efficacy of this approach is evidenced in Table 3, which presents the statistical indicators of the data both pre- and post-interpolation. Notably, while the post-interpolation data retains a close resemblance to the original data in terms of statistical indicators, it is important to acknowledge that interpolated data are not independent observations. The validity of the interpolation method, therefore, depends on the specific application and context. In this study, interpolation was used to address missing variables, and we ensure that

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the statistical properties of the original data were preserved to the greatest extent possible. This approach allows us to maintain the integrity of our analyses while recognizing the inherent limitations of using interpolated data.

Upon visualizing the values of the three NPP products (VGPM, CbPM, and CAFE) (Fig. 3), it became evident that each exhibits a distinct periodicity, with the fluctuation ranges remaining stable yet markedly varied among them. Specifically, VGPM NPPs are the smallest, followed by CAFE NPPs, while CbPM NPPs have the largest values. To elucidate the correlation between these NPP products and our dataset, we generated Pearson correlation plots (Fig. 4). The results revealed that the variables with the highest correlations differed among the three NPP values. Notably, VGPM NPP showed the strongest correlation with SST, because the estimation of VGPM NPP is directly dependent on the optimal assimilation efficiency of the productivity profile (Behrenfeld et al., 1997). Whereas both CAFE NPP and CbPM NPP were most closely correlated with AP, albeit in opposing directions—CAFE NPP displayed a positive correlation and CbPM NPP, a negative one. Changes in AP mainly affect atmospheric stability, cloudiness, and precipitation, which in turn indirectly affect light conditions in the ocean and phytoplankton photosynthesis. Photosynthesis in plants may be inhibited under low-pressure environments. This analysis highlights that the three NPP estimation models exhibit distinct affinities with each variable. In summary, among the three models, VGPM NPP possesses the most significant correlation with the variables, followed by CAFE NPP, and lastly CbPM NPP.

2.2. Methods

2.2.1. Bayesian Probability Prediction

Bayesian models can adeptly quantify the uncertainty in the distribution of predicted outcomes. The Bayesian approach is particularly advantageous in scenarios with limited training data or when potential invisibility in training data cannot be discounted in practical applications (Perfors et al, 2011). The Bayesian formula is represented as:

$$P(\theta|D) = \frac{P(D|\theta) \cdot P(\theta)}{P(D)} \#(1)$$

where $P(\theta|D)$ denotes the posterior probability, $P(D|\theta)$ the likelihood probability, $P(\theta)$ the prior probability, and $P(D)$ the marginal probability for normalization.

When a training dataset D is available, the probability distribution $P(\theta|D)$ of θ is computable using the aforementioned Bayesian formula (Dürr et al, 2020). To deduce $P(\theta|D)$, it is imperative to ascertain the likelihood probability $P(D|\theta)$ of the observed data under the model parameter θ. $P(D|\theta)$ can also be interpreted as the probability of obtaining the training dataset D given parameter θ. Additionally, knowledge of the prior probability $P(\theta)$ and the evidence $P(D)$ is essential. Given that the training dataset D is fixed, $P(D)$ remains constant. Consequently, the posterior distribution is proportional to the likelihood probability multiplied by the prior distribution, i.e., $P(\theta|D) \propto P(D|\theta) \cdot P(\theta)$, in accordance with Bayes' Law.

In this study, the Bayesian approach is employed to calculate the posterior distributions of the parameters considering the prior information and the input data. Subsequent predictions are made using the posterior distributions, yielding a probability distribution for each predicted value. Ultimately, the model's ability to estimate the uncertainty in the NPP is illustrated by plotting the prediction ranges for different targets and comparing them to actual observations.

2.2.2. Neural Network Probabilistic Prediction Model Based on TFP

TensorFlow Probability (TFP) represents a sophisticated library of statistical algorithms, devised atop the TensorFlow Python API. Its primary objective is to streamline the integration of probabilistic models with deep learning frameworks. TFP offers a comprehensive suite of tools, enabling the construction of probabilistic

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models adept at estimating uncertainty. Aiming to thoroughly assess the predictive efficacy of the three NPP products, we employed a neural network model grounded in the TFP framework, capitalizing on its versatility and potent expressive capabilities for probabilistic prediction in marine ecosystems.

The architecture of this neural network model incorporates multiple hidden layers, each implementing a nonlinear transformation via an activation function. Such a configuration enables the model to automatically extract higher-order features and intricate patterns from the data. Our selection of TFP as the implementation medium allows us to model the neural network's output by integrating probability distributions, thus addressing the model's uncertainty regarding predictions and yielding more exhaustive insights. Specifically, our neural network model utilizes a distribution layer in the output stage, producing a probabilistic distribution concerning the target variable, as opposed to a mere deterministic point prediction. This probabilistic output facilitates the quantification of the model's confidence level for each prediction, extending beyond mere point estimates.

The integration of Bayesian models and probabilistic neural networks in our approach addresses key challenges in the remote sensing of NPP. These challenges include handling the variability and uncertainty inherent in satellite-derived data and environmental factors, thus improving the robustness of NPP estimates. In this study, the input variables for the models are the 11 environmental variables mentioned in Section 2.1, and the outputs are VGPM, CbPM, and CAFE NPPs. The selection of input data was not limited to variables directly related to phytoplankton photosynthesis, such as SST, PAR, and SH. Instead, it also included a wide range of environmental variables that could influence phytoplankton growth, such as TH, WS, and AP, which are physical dynamics and meteorological characteristics. Since phytoplankton are the primary source of NPP, environmental factors affecting phytoplankton growth also indirectly impact NPP. The dataset spans 4,077 days, but due to the 8-day time interval of the downloaded NPP products, only 514 complete

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datasets are available for model training and performance evaluation. Given the limited amount of data, 80% of the 514 sets are used for model training and parameter tuning, while the remaining 20% are used for performance evaluation. In the neural network probabilistic prediction model, there are six layers, with two output nodes used to estimate the mean and standard deviation. The Gaussian distribution is employed in the distribution layer, and the loss function is the negative log-likelihood loss function. The detailed parameters of the neural network are presented in Table 4.

2.3. Model Evaluation

Prior to model evaluation, we normalized the NPP satellite data. This step is critical to improving model performance because it removes the potential effects of different data scales, allowing the model to consider each data point more fairly. Normalization ensures that the distribution range of NPP data has the same weight during model training, thus improving the model's ability to capture the inherent patterns and features of the data. In addition, normalization helps reduce the noise and bias introduced by data scale differences, further enhancing the stability and predictive accuracy of the model.

Before training the model, we divided the dataset reasonably. Specifically, we divided the dataset into 80% training set and 20% testing set. This division aims to ensure that the model can fully learn the features and patterns of the data during the training process, while retaining enough independent data for testing the predictive ability of the model. This way of dividing the dataset helps us to evaluate the performance of the model more accurately and avoid problems such as overfitting.

2.3.1. CRPS

Continuous Ranked Probability Score (CRPS) is a sophisticated statistical metric employed to evaluate the efficacy of forecasting models. Initially introduced in the 1970s (Matheson & Winkler, 1976), CRPS is widely utilized in areas such as weather

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forecasting (Zamo et al., 2018). It quantifies the divergence between the predicted probability distribution and the actual observations (Hersbach, 2000). Ideally suited for scenarios where the target variable is continuous and the model predicts its distribution (Pic et al., 2023), CRPS equates to the mean absolute error (MAE) in deterministic forecasting (Zhao et al., 2015).

In probabilistic forecasting, the focus extends beyond mere point estimates to encompass the shape and dispersion of the probability distribution. Hence, traditional scoring functions prove inadequate, as aggregating the predicted distributions into their mean or median neglects critical information about the dispersion and shape. CRPS, by embracing the entire probability distribution, emerges as an invaluable tool in assessing model uncertainty. CRPS is calculated as follows:

1. For each sample, calculate the discrepancy between the cumulative distribution function (CDF) of the predicted and observed values.

2. Aggregate the variances for all samples and divide by the number of samples to obtain the average variance.

$$CRPS(F, x) = \int_{-\infty}^{+\infty} [(F(y) - H(y - x)]^2 dy \qquad (2)$$

$$CRPS = \frac{1}{n} \sum_{i=1}^{n} CRPS(F_i, x_i) \qquad (3)$$

where $F(y)$ denotes the CDF of the predicted value, y the predicted value, x the observed value, and $H(y\text{-}x)$ the Heaviside function which is 0 when $y<x$ and 1 otherwise. n indicates the total number of samples, and CRPS (F_i, x_i) the CRPS value for the *i-th* sample.

A smaller CRPS value signifies a closer alignment of the model's probability distribution with actual observation, integrating insights on both the shape and location of the distribution and demonstrating sensitivity to outliers. Unlike other

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metrics such as Root Mean Square Error (RMSE) or Mean Absolute Error (MAE), CRPS offers a more holistic evaluation of a probability distribution's predictive capacity by considering the full distribution shape. For Bayesian and neural network models, comparing CRPS values facilitates an understanding of their proficiency in fitting the entire probability distribution.

2.3.2. RMSD

Root Mean Squared Deviation (RMSD) is a widely recognized evaluation metric in regression analyses, primarily employed to quantify the discrepancy between a model's predicted values and the actual observed values. Characterized by its intuitive nature and simplicity in computation, RMSD is particularly beneficial in scenarios where emphasis is placed on the magnitude of difference between predicted and actual values, irrespective of the difference's direction.

$$RMSD = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \tag{4}$$

where n denotes the number of samples, y_i represents the actual value of the *i-th* sample, and $\hat{y}_i$ symbolizes the predicted value of the *i-th* sample.

A lower RMSD value is indicative of superior model performance, signaling a smaller variance between the model's predictions and the observed values. Nevertheless, it is important to note that RMSD exhibits sensitivity to outliers, as it constitutes the mean of the squared differences. Incorporating RMSD alongside CRPS in our analysis enables a more comprehensive evaluation of both the overall accuracy and uncertainty inherent in the predictions.

2.3.3. MAPD

Mean Absolute Percentage Deviation (MAPD) is a frequently utilized percentage error metric in regression problems. It expresses the prediction error as a percentage, offering an insightful perspective into the relative error between predicted results and

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true values in predictive model evaluations.

$$MAPD = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{\hat{y}_i - y_i}{y_i}\right| \times 100\% \tag{5}$$

where n signifies the number of samples, y_i the actual value of the *i-th* sample, and $\hat{y}_i$ the predicted value of the *i-th* sample.

A lower MAPD value is desirable, indicating a reduced relative error of the model. However, a cautionary note: MAPD may prove unreliable in instances where the predicted value approaches zero, as a zero denominator results in infinity. Therefore, careful consideration is warranted when employing MAPD, particularly in scenarios where relative accuracy is paramount.

In the context of comparing Bayesian probabilistic prediction models with neural network probabilistic prediction models, the synergistic application of these three metrics — CRPS, RMSD, and MAPD — affords a multifaceted assessment of the models. This triad of metrics enhances our understanding of the importance of relative error alongside the accuracy of point estimates and the fit of probability distributions.

3. Results and Discussion

3.1. Comparative Analysis of Prediction Efficacy Between Two Models

We utilized VGPM, CbPM, and CAFE NPPs as prediction targets to scrutinize the predictive effectiveness of both the neural network-based probabilistic prediction model and the empirical distribution-based Bayesian probabilistic prediction model. Fig. 5 presents a comparison of CRPS, RMSD, and MAPD values for these models across training and test datasets. Notably, CRPS provides a holistic evaluation of prediction accuracy and reliability. All the metrics are calculated using normalized data for better comparison. Lower values are indicative of enhanced model performance. Fig. 5(a)-(c) and (d)-(f) respectively depict the CRPS, RMSD, and MAPD of the NN model and Bayes model when using the three NPP values as

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prediction targets. The color blue represents the training set, while red represents the test set. It can be observed from Fig.5 (a) and (d) that the CRPS values of both the NN model and Bayes model are similar. When VGPM NPP is used as a prediction target, the performance of the models is closest between the training set and test set, followed by CbPM NPP. However, CAFE NPP has the lowest CRPS value among all three models, with its test set slightly larger than that of its training set.

In terms of RMSD metrics (Fig. 5 (b) and (e)), when VGPM NPP is used as a prediction target, its index value is significantly higher compared to others; however, its performance between training set and test set remains close. When CbPM NPP is used as a prediction target, Bayes model outperforms NN model but exhibits a larger difference between training set and test set compared to NN model.

On using CAFE NPP as a prediction target, both models show more consistent performance. The values of these indicators are relatively close in all aspects at around 0.2. Regarding MAPD metrics (Fig.5 (c) and (f)), clear differences among the three NPP models can be seen where CAFE has obviously lower index value compared to CbPM and VGPM. In addition, for NN model's MAPD index value for CAFE is lower than that for Bayes model. However there exists significant difference between its training set and test set.

Overall evaluation indicates that under both models' assessment criteria, CAFE NPP demonstrates superior accuracy in predicting effects compared to VGPM NPP and CbPM NPP. VGPM NPP shows greater instability with inferiority in it's trainig process over testing process (Fig.5 (d), (e), (f)), which may be attributed to overfitting. However, there is a more noticeable difference in the performance of CbPM NPP in the two models. The CRPS value and RMSD value in the Bayes model are significantly lower than those in the NN model (Bayes is less than 0.2, while NN is more than 0.2). Therefore, the following analyses will focus on the efficacy of probabilistic prediction models with CAFE NPP as the prediction target.

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3.2. Quantify the Uncertainty of CAFE NPP

When quantifying uncertainty in the CAFE NPP, we need to focus on the uncertainty factors that exist in the input variables in addition to the uncertainty that may arise during model training. These uncertainty factors include measurement errors and temporal variability, among others. Measurement errors usually originate from the accuracy limitations of the instruments, the complexity of the observation environment, or the instability of human operations. These errors not only affect the accuracy of the input variables to varying degrees, but also propagate through the model and thus affect the accuracy of the prediction results. The temporal variability, on the other hand, reflects the dynamic changes of marine environmental parameters, such as seasonal temperature changes, cyclic fluctuations of tides, etc., which also affect the NPP prediction results. Consequently, quantifying these uncertainties is particularly important in conducting CAFE NPP predictions.

3.2.1. Comparative Analysis of Confidence Interval Widths

Fig. 6 illustrates the comparison between the forecast mean of the NN model and Bayes model, and the CAFE NPP value when CAFE NPP is utilized as the prediction target. In the figure, the triangular icons represent 514 sets of the forecast average, while the gray and blue represent the 95% and 75% confidence intervals, respectively. Overall, both models exhibit relatively wide confidence intervals for their predicted results, possibly due to the large range of changes in CAFE NPP. The models may face greater challenges in capturing this wide range of changes, resulting in increased uncertainty.

When CAFE NPP is less than 450 mg C m^{-2} d^{-1}, both models tend to overestimate the actual NPP value. This phenomenon becomes more pronounced when CAFE NPP is less than 350 mg C m^{-2} d^{-1}. In contrast, a certain linear relationship between true value and predicted mean value emerges within a range of 450-600 mg C m^{-2} d^{-1}. Most of the predicted mean values are distributed around the 1:1 line in this range, indicating higher accuracy by these models. However, when

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CAFE NPP exceeds 600 mg C m^{-2} d^{-1}, it is observed that both models tend to underestimate actual NPP values. This phenomenon may be attributed to an imbalance in sample data distribution within different intervals of CAFE NPP. The majority of data points are concentrated in a narrow range (350-600 mg C m^{-2} d^{-1}), while data points in other intervals are scarce. This inadequacy makes it difficult for model training to capture its distribution law accurately and leads to increased prediction uncertainty within these ranges.

Compared with the two models, the predicted value of NN model is more concentrated around the 1:1 line, while the predicted value of Bayes model is relatively dispersed and the confidence interval is wider. The smaller the confidence interval width, the higher the accuracy of model prediction. It manifests that the NN probabilistic prediction model is more accurate in predicting CAFE NPP than the Bayes probabilistic prediction model, and the uncertainty of its prediction results is lower. The prediction mean obtained by the NN probabilistic prediction model is closer to the 1:1 line, which usually means that the deviation between the predicted value of the model and the actual observed value is small, that is, the prediction accuracy of the model is higher. The differences in the performance of the two models may stem from their different strategies for dealing with uncertainty and data fitting. Neural network models typically capture the nonlinear relationships of data through a large number of parameters and complex network structures, so they may be able to fit the data distribution more accurately in some cases. Bayes model deals with uncertainty by introducing prior knowledge and a posteriori inference, but its performance may be limited under some complex data distributions.

To further elucidate the models' effectiveness in probabilistic prediction of CAFE NPP, Fig. 7 visualizes the time series model predictions with a 95% confidence interval uncertainty range. The figure shows that almost all CAFE NPP values fall within the 95% confidence interval of the mean of the predicted values. It can be clearly seen that the predicted distribution of the NN model is much smaller than that of the Bayes model, which is consistent with the results shown in Fig. 6. The NPP is

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clearly periodic in time, and both models are able to align their predictions on the test set with the periodicity of the training set. In particular, the scatter in the NN model is more centrally distributed around the red line, while the scatter in the Bayes model is more discrete from the red line, which further suggests that the NN model has a more accurate estimate in predicting the CAFE NPP.

Overall, the trends in the predicted means of the two models are consistent with the trends in the majority of CAFE NPP values, which further validates the accuracy of the two methods in capturing the process of CAFE NPP changes. This consistency not only indicates that the models can accurately reflect the long-term trends of CAFE NPP changes, but also capture short-term fluctuations and outliers. This is of great significance for ecosystem monitoring and prediction, and helps to better understand the dynamics of the ecosystem and take appropriate management and conservation measures. However, in terms of confidence interval width, the width of the 95% confidence interval in the results of the Bayesian probabilistic prediction model is larger than that of the neural network probabilistic prediction model, indicating that the Bayesian probabilistic prediction model is not as sharp as the neural network probabilistic prediction model, which is more locally sensitive and able to respond to the changes in data more quickly.

Although the neural network probabilistic prediction model shows an advantage in terms of sharpness and local sensitivity, this does not mean that it is superior to the Bayesian model in all cases. In fact, Bayesian models are more robust and explanatory by introducing prior knowledge and posterior inferences to deal with uncertainty. Therefore, when choosing a predictive model, trade-offs need to be made based on specific application scenarios and data characteristics.

3.2.2. Comparative Analysis of CDF

Evaluating the empirical CDF of the model input data and the average predictive CDF affords a graphical representation of the model's predictive accuracy. A higher degree of overlap in the CDF curves signifies greater similarity between the two distributions, thereby reflecting superior model predictions. Fig. 8 depicts the overall

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predictive distribution versus the empirical distribution of the CAFE NPP input data. Concurrently, Fig. 9 methodically quantifies the disparity between the average predictive CDF and the empirical CDF of the input data. Optimally, the divergence between these two CDFs should be minimal, manifested as extensive overlap between the yellow and blue curves in Fig. 8, and the blue curve in Fig. 9 approaching zero. Fig. 8 demonstrates the CDF curves of the predicted mean values after the normalization process and the CDF curves of the CAFE NPP. The CDF plots of the normalized data can reflect the statistical distribution of the datasets, especially when the different datasets have different magnitudes or scales, and the normalization can eliminate these differences, which makes the comparisons and analyses between the different datasets more accurate and intuitive. Fig. 9 specifically quantifies the difference between the two CDF curves in FIG. 8 at each point, which is accomplished by calculating the difference between the y-values of the two CDF curves at the same x-value.

Observing the results in the figure, it is found that the mean values of the prediction results of the NN probabilistic prediction model and the Bayes probabilistic prediction model are roughly consistent with the trend of the CDF of the input prediction target CAFE NPP. For the NN probabilistic prediction model, when the CAFE NPP is small, the two CDF curves on the training set and the test set move gently and almost overlap, with the difference close to 0, which indicates that the model can predict the actual data distribution well within the range of small values of CAFE NPP. As CAFE NPP increases, the difference between the CDF curves starts to become larger, and the predicted mean CDF on the training set lies below the CAFE NPP CDF, with the difference between the two ranging from 0 - 0.2. The predicted mean CDF on the test set first lies below the true value CDF curve, and then becomes steeper and lies above the true value CDF curve, and when CAFE NPP continues to increase, the two curves alternate again, which may imply that the model is more unstable in predicting high values, and the absolute value of the difference between the CDF does not exceed 0.1.

For the Bayesian probabilistic prediction model, the predicted mean CDF curve is above the true value in the training set. When the CAFE NPP increases to a certain extent, the two curves alternate, and the absolute value of the difference between the CDF does not exceed 0.2. In the test set, the two CDF curves overlap first and then separate. The predicted mean CDF rises more quickly, and is on top of the true value CDF curve, with the difference between the two curves not exceeding 0.1 when the CAFE NPP increases to a certain extent. When the NPP increases to a certain degree, the two curves overlap again, and the absolute value of the difference between the CDF does not exceed 0.3. Overall, the difference between that of the predicted mean values and the CDF of the true values obtained by the two models is small, which indicates that the overall deviation of the model predictions is not large, and both models show good prediction performance and can capture the statistical characteristics of the data well. However, the CDF curves of the neural network probabilistic prediction model are closer to the true values on both the training and test sets, possibly implying that the neural network model is more effective in dealing with complex data and capturing nonlinear relationships. The flexibility of neural networks allows them to adapt to different data distributions and patterns.

Table 5 presents RMSD, MAPD, and CRPS for both models. Additionally, we analyzed the proportion of raw input data encompassed within the 95% confidence interval, thereby providing a more nuanced evaluation of the model's proficiency in capturing CAFE NPP uncertainty. According to Table 5, the neural network-based probabilistic prediction model exhibits superior performance in terms of CRPS, RMSD, and MAPD. This denotes a higher level of accuracy and reliability for the neural network model in probabilistic predictions of CAFE NPP, especially when considering uncertainty. Conversely, the Bayesian probabilistic prediction model demonstrates a stronger ability to encompass a greater proportion of the raw input data within the 95% confidence interval. This suggests that while it may exhibit higher overall uncertainty, it has a more pronounced capability to capture the nuances of uncertainty.

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This comparative analysis elucidates that both the neural network-based probabilistic prediction model and the Bayesian probabilistic prediction model, grounded in empirical distributions, are adept at capturing and quantifying the uncertainty of CAFE NPP. While the Bayesian model demonstrates a heightened capability in encompassing a broader scope of uncertainty, the neural network model distinguishes itself by its superior accuracy and reliability, particularly in precisely predicting the uncertainty of CAFE NPP. A notable observation is that when CAFE NPP values exceed 350 mg C m^{-2} d^{-1}, the predictive performance of both models deteriorates. This manifests as an underestimation of mean predictions, indicating an inability to fully and accurately predict NPP across the entire range of size classes. The underlying reason for this may stem from the considerable variation in the input data and its skewed sample distribution. Most notably, a significant proportion of the samples were primarily concentrated within the 200-350 mg C m^{-2} d^{-1} range. In contrast, CAFE NPP values exceeding 350 mg C m^{-2} d^{-1} constitute only 28% of the input dataset. Consequently, the models exhibit insufficient learning of higher value ranges during the training phase, resulting in a notable prediction bias for larger CAFE NPP values.

3.3. Probabilistic Prediction of NPP in Weizhou Island (2007–2018)

Given the 8-day temporal resolution of data acquired by remote sensing satellites and the consequent data incompleteness, this study employed the previously trained neural network and the Bayesian probabilistic prediction models to forecast the daily NPP in the Weizhou Island sea area from 2007 to March 2018, thereby supplementing the NPP dataset. The results are illustrated in Fig. 10, where the predicted mean values and 95% confidence intervals for both models are displayed. Fig. 10(c) reveals that the Bayesian model's confidence interval is broader, primarily due to its lower limit, yet no substantial difference is noted between the predicted mean values of the two models. Both models effectively mirror the trend of NPP. The analysis of the annual change of NPP shows a clear periodicity, which means that the change of NPP

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is not random, but follows certain laws and patterns. Combined with Fig. 11, the seasonal variation of NPP throughout the year emerges. Specifically, NPP shows a decreasing trend from January to July each year, with July generally being the lowest level of the whole year. Then it increases from July to November and slightly decreases from November to December. Overall, NPP has larger values in winter and spring. These results provide important insights into seasonal variations and interannual trends of NPP in the Weizhou Island waters and provide valuable data to support the study of the marine ecosystem dynamics.

However, the significance of our work extends far beyond mere data replication. The primary aim of our study is to enhance the reliability of marine NPP estimates by using advanced probabilistic models. Our objective extends beyond merely reproducing satellite NPP products. We aim to improve the overall accuracy and uncertainty quantification of NPP estimates by incorporating a robust probabilistic framework. This framework helps to better understand and quantify the uncertainties inherent in marine NPP, whether they originate from satellite data or environmental factors. By using Bayesian models and probabilistic neural networks, we not only replicate satellite NPP estimates but also capture and quantify uncertainties at multiple levels. These models account for uncertainties in the satellite products, input data variability, and the predictive model itself, thus providing a more comprehensive uncertainty quantification relevant to marine NPP.

4. Conclusion

This study primarily addresses the challenge of uncertainty in satellite ocean color data estimates of ocean NPP. Departing from traditional point estimation regression models, we embraced a probabilistic prediction approach where the output is a probability distribution. The models utilized in this study include a Bayesian probabilistic prediction model based on empirical distributions and a deep learning-based probabilistic prediction model under the TFP framework. Focusing on the NPP uncertainty analysis in the Weizhou Island sea area, we explored the effect of the probabilistic prediction model when the NPPs obtained by the VGPM, CbPM, and CAFE methods, respectively, are used as the prediction targets. Furthermore, this study compares and analyzes the capabilities of Bayesian and neural network probabilistic models in predicting the CAFE NPP uncertainty. The results reveal that both models are competent in quantifying CAFE NPP uncertainty.

When exploring the uncertainty of the NPP using the Bayesian probabilistic prediction model and the neural network probabilistic prediction model, the results show that the two probabilistic prediction models are the most effective when the prediction target is the CAFE NPP. The probability distributions obtained by the two probabilistic prediction models are similar to those of CAFE NPP, with the difference in CDF between the predicted mean and true values at each data point not exceeding 0.2 for the neural network probabilistic prediction model and 0.3 for the Bayesian probabilistic prediction model. In contrast, the confidence intervals for the outputs of the Bayesian probabilistic prediction model are wider, and the proportion of the CAFE NPP that falls in the confidence intervals is higher, which shows that Bayes is more capable of capturing uncertainty, but its accuracy is not high. However, the neural network probabilistic prediction model is more accurate and reliable. Its performance is better in many assessment indicators, but not all CAFE NPP values in the size range can be predicted accurately by the model. When the CAFE NPP is less than 450 mg C m^{-2} d^{-1}, the model tends to overestimate the actual NPP value. When CAFE NPP is larger than 600 mg C m^{-2} d^{-1}, it tends to underestimate the actual NPP value. When the two probabilistic prediction models are applied to the prediction of CAFE NPP in the Weizhou Island waters between January 2007 and February 2018, the prediction results illustrate the interannual trend of CAFE NPP, and the magnitude of NPP is found to show obvious cyclic changes. Our study demonstrates the novel application of advanced probabilistic models to the remote sensing of marine NPP. By addressing the uncertainties in satellite-derived estimates and improving the reliability of NPP predictions, our work contributes to advancing the field of marine remote sensing and provides a foundation for future research.

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In the context of ongoing climate change, accurately capturing and reducing the uncertainty of marine NPP emerges as a pivotal research focus in marine ecology. This endeavor is crucial for a deeper understanding of energy and matter flow in marine ecosystems, providing a solid scientific foundation for the judicious management of the conservation of natural resources. While our study has advanced the field by demonstrating the feasibility of probabilistic prediction in quantifying NPP uncertainty, we acknowledge the potential for further enhancements and expansions. Looking ahead, future research could embark on the following paths to augment our work: (1) Expanding the research scope: The current study has concentrated primarily on specific marine areas. Future initiatives could broaden this focus to encompass diverse geographic regions and types of marine ecosystems. Such expansion is vital to gain a more comprehensive understanding of probabilistic prediction's applicability and effectiveness across varying environmental conditions; (2) Enhancing data collection: The acquisition of more extensive and comprehensive observational data is instrumental in refining model training and prediction accuracy. Future endeavors should aim to amass a richer array of observational data, emphasizing the need for long-term time series and high-resolution remote sensing data. These efforts will significantly bolster the development and validation of robust probabilistic prediction models; (3) Refining model structure: Our study utilized Bayesian probabilistic regression and deep learning-based probabilistic prediction models. Future studies could explore the integration of other advanced model structures or the optimization of the existing ones, aiming to elevate the model's performance and robustness. Through these concerted efforts, we aspire to continually refine the methodologies of probabilistic prediction in quantifying marine NPP uncertainty, thereby laying the groundwork for more precise ecosystem management and environmental protection strategies.

Author contribution Statement

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Supervision, Funding acquisition.

Mengyu Xie: Conceptualization, Methodology, Data Curation, Writing - Original Draft, Visualization.

Yanqun Lu: Conceptualization, Methodology, Data Curation, Writing - Original Draft, Visualization.

Liwei Sun：Data Curation, Supervision,Funding acquisition.

Na Liu: Writing - Review & Editing, Supervision.

Han Qiu: Writing - Review & Editing, Supervision.

Dongdong Liu: Writing - Review & Editing, Supervision.

Chuanhao Wu: Writing - Review & Editing, Supervision.

Pan Wu: Writing - Review & Editing, Supervision.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Tables

Table 1. Summary of Variables and Data Sources.

Variable name	Variable description	Data source
SST	Sea surface temperature (°C)	
Sal	Salinity (‰)	
TH	Height of tide(m)	
AP	Air pressure (hPa)	Weizhou Marine environment monitoring station
RH	Relative humidity (%)	
SV	Sea visibility (km)	
WS	Wind speed ($m \cdot s^{-1}$)	
H/10	1/10th significant wave height (m)	
PAR	Photosynthetically active radiation ($W \cdot m^{-2}$)	https://oceancolor.gsfc.nasa.gov/
SSP	Sea surface precipitation (mm)	https://www.earthdata.nasa.gov/
SH	Sunshine hours ($h \cdot d^{-1}$)	https://data.cma.cn/
VGPM NPP	NPP from the VGPM model (mgC $m^{-2} \cdot d^{-1}$)	
CbPM NPP	NPP from the CbPM model (mgC $m^{-2} \cdot d^{-1}$)	http://orca.science.oregonstate.edu/npp.visual.php
CAFE NPP	NPP from the CAFE model (mgC $m^{-2} \cdot d^{-1}$)	

Table 2. Summary of Missing Variables.

Variable	SV (km)	H/10 (m)	PAR ($W \cdot m^{-2}$)	SSP (mm)	SH ($h \cdot d^{-1}$)
Missing quantity	31	51	828	378	18

Table 3. Statistics of data pre- and post-interpolation.

	SV (km)		H/10 (m)		PAR ($W \cdot m^{-2}$)		SSP (mm)		SH ($h \cdot d^{-1}$)	
	pre-	post-	pre-	post-	pre-	post-	pre-	post-	pre-	post-
count	4046	4077	4026	4077	3249	4077	3699	4077	4059	4077
mean	15.22	15.23	0.57	0.57	34.92	35.97	4.94	4.85	5.19	5.18
std	10.33	10.30	0.41	0.41	15.64	15.20	16.13	15.61	3.93	3.93

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min	0.00	0.00	0.00	0.00	1.20	1.20	0.00	0.00	0.00	0.00
25%	7.00	7.00	0.30	0.30	22.19	24.14	0.00	0.00	0.80	0.80
50%	12.00	12.00	0.50	0.50	36.03	36.87	0.00	0.00	5.60	5.60
75%	25.00	25.00	0.70	0.70	47.58	48.49	1.30	1.50	8.90	8.80
max	50.00	50.00	4.00	4.00	61.13	61.13	280.40	280.40	12.6	12.6

Table 4. Parameters of the Neural Network Model

	Hyper-parameters	
Layer Sizes	Layer 1	64
	Layer 2	32
	Layer 3	16
	Layer4	16
	Layer 5	2
	Distribution Layer	Gaussian distribution
Epochs	800	
Learning Rate	0.0001	
Batch Size	16	
optimizer	Adam	
loss	Negative log likelihood	

Table 5. CRPS, RMSD, MAPD, and proportion of input data within 95% confidence interval.

	CRPS		RMSD		MAPD		Proportion	
	Train	Test	Train	Test	Train	Test	Train	Test
NN	0.096	0.133	0.149	0.198	11.828	13.237	0.971	0.932
Bayes	0.151	0.20	0.201	0.253	13.909	14.145	0.976	0.951

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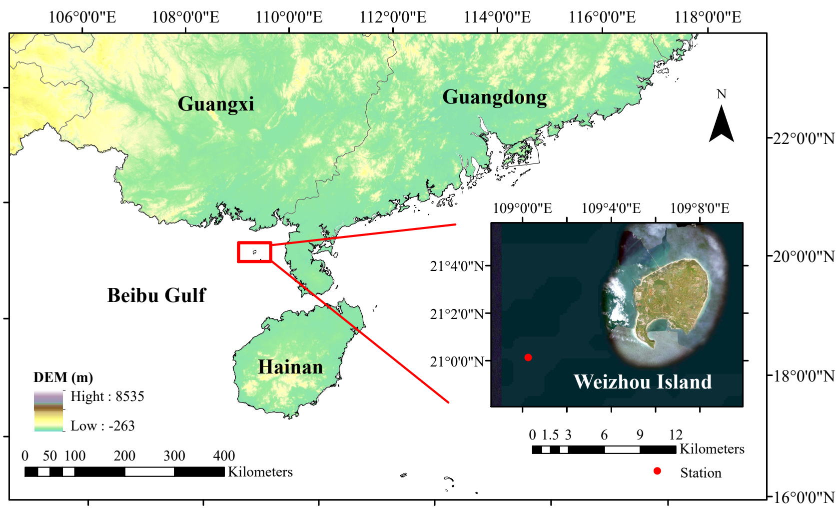
790 # Figures



791

792 **Fig. 1.** The research area is located in the waters of Weizhou Island in Beibu Gulf, south China.
793 The red dots in the figure indicate the location of Weizhou Marine Environmental Monitoring
794 Station (21.0017°N, 109.0117°E). Eight distinct sets of monitoring data were collected from this
795 monitoring station.

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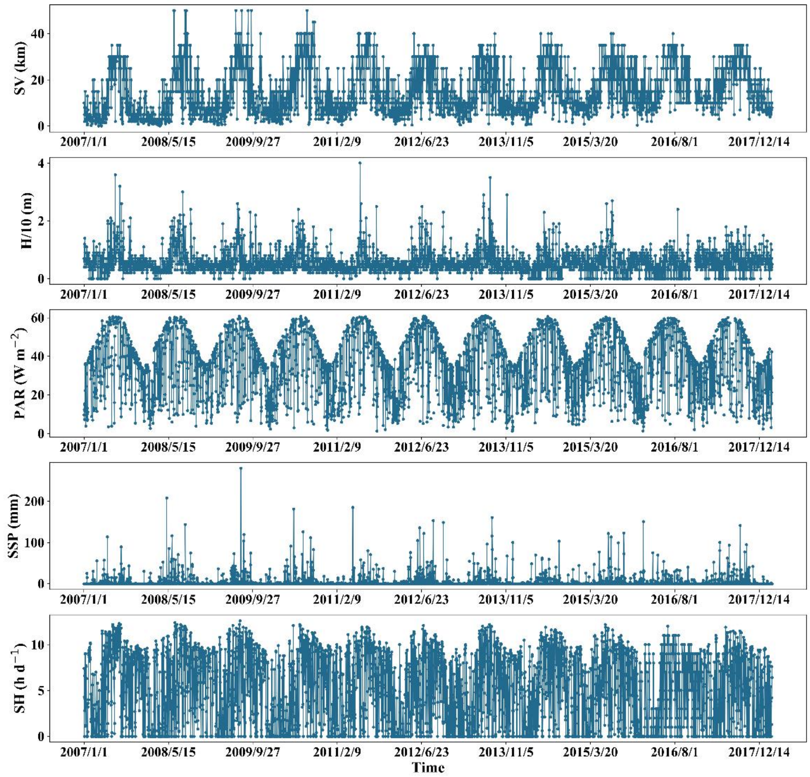

Fig. 2. Time series plots of SV, H/10, PAR, SSP, and SH with missing variables, showing the cyclical variation of these five variables.

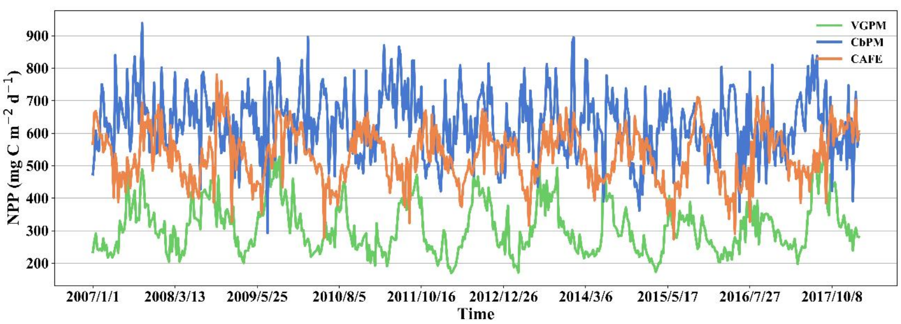

Fig. 3. Time series of VGPM, CbPM, and CAFE NPPs from January 2007 to February 2018, where the green line represents VGPM NPP, the blue line represents CbPM NPP, and the orange line represents CAFE NPP. Abbreviations and data sources can be referenced in Table 1.

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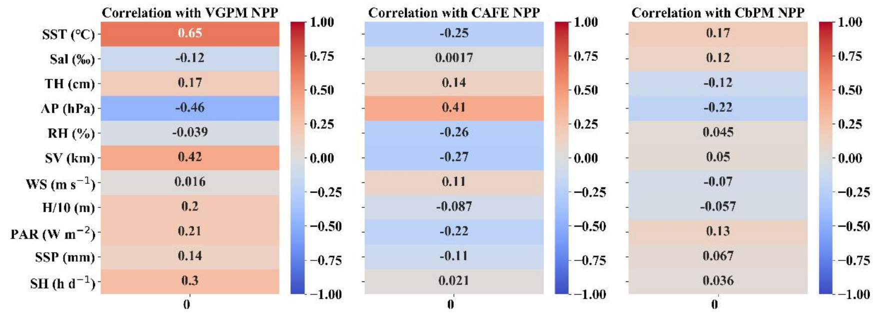

Fig. 4. Pearson correlation of VGPM, CAFE, and CbPM NPPs with input variables. The deeper the shade of red indicates a stronger positive correlation, whereas the deeper shade of blue indicates a stronger negative correlation.

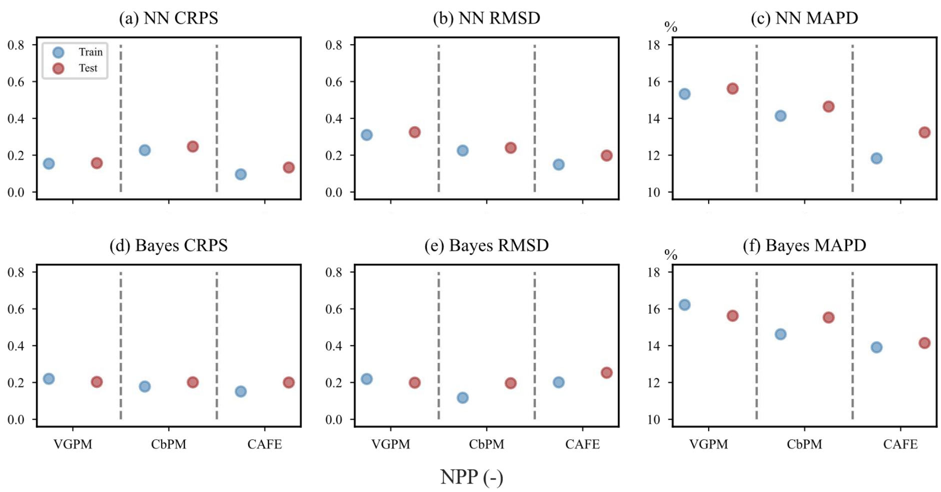

Fig. 5. Comparison of NPP predictive effects from VGPM, CbPM, and CAFE. Panels (a)–(c) present the results from the neural network-based probabilistic prediction models; panels (d)–(f) the results from Bayesian probabilistic prediction models based on empirical distributions. The horizontal coordinates represent the VGPM, CbPM, CAFE NPPs as inputs in sequence, separated by gray dashed lines, where blue dots represent data from the training set, and red dots denote data from the test set, and the vertical coordinates are the values of the three metrics, CRPS, RMSD, MAPD. Since NPP values were normalized to the range of 0 – 1, the y axes of subplots (a), (b), (d), and (e) are dimensionless. The units for MAPD are percentile.

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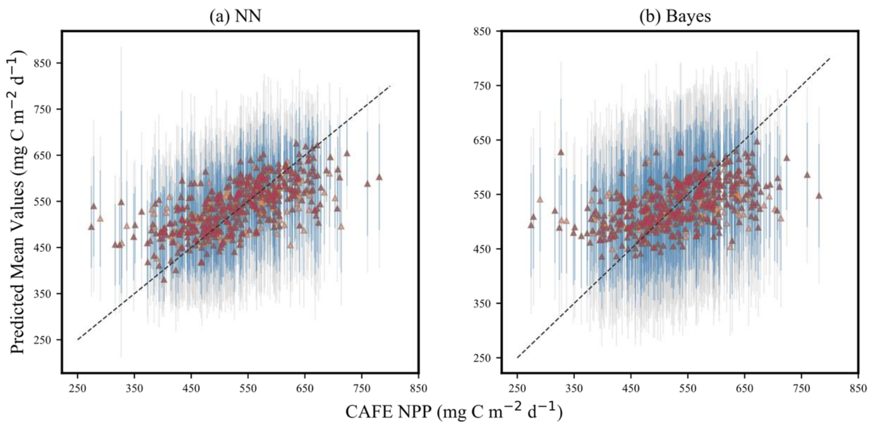

Fig. 6. Uncertainty quantification of (a) neural network-based probabilistic prediction model and (b) empirical distribution-based Bayesian probabilistic prediction model. The horizontal axes represent the input VGPM NPP value, while the vertical axes show the mean predicted by the model. The triangular icons in the figure represent 514 sets of the forecast average, the gray vertical lines represent the 95% confidence intervals for the predictions, and the blue vertical lines represent the 75% confidence intervals.

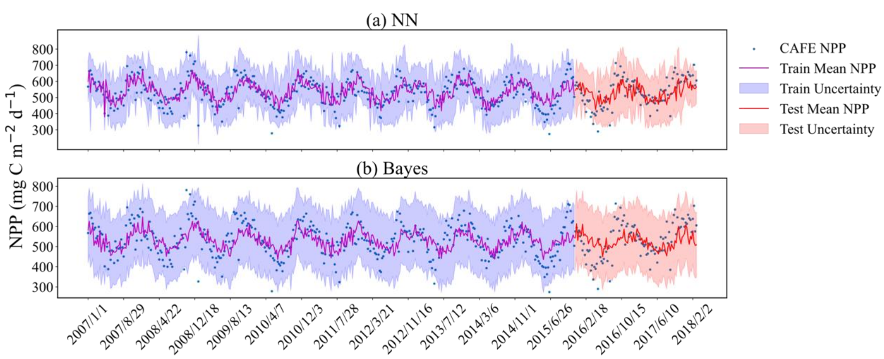

Fig. 7. Comparison of original and predicted mean values shown at an 8-day temporal resolution within a 95% confidence interval. (a) Probabilistic prediction results based on neural networks; (b) Bayesian probabilistic prediction results based on empirical distributions. The dashed lines represent the mean values of the probabilistic predictions. The purple and red shaded areas illustrate the uncertainty ranges for the training and the test sets, respectively. Blue dots signify observed data points. All predictions and observations are presented in chronological sequence.

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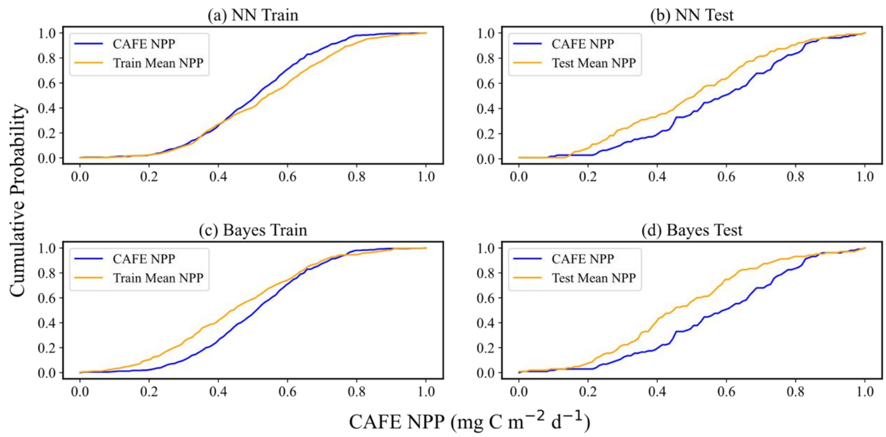

Fig. 8. Comparison of VGPM NPP and predicted mean CDF. Panels (a) and (b) display the performance of the training and test sets, respectively, in the neural network-based probabilistic prediction model. Panels (c) and (d) illustrate the performance of the training and test sets, respectively, in the empirical distribution-based Bayesian probabilistic prediction model. In each panel, the blue curves represent the CDFs of the VGPM NPP values, while the yellow curves depict the CDFs of the model's predicted mean values.

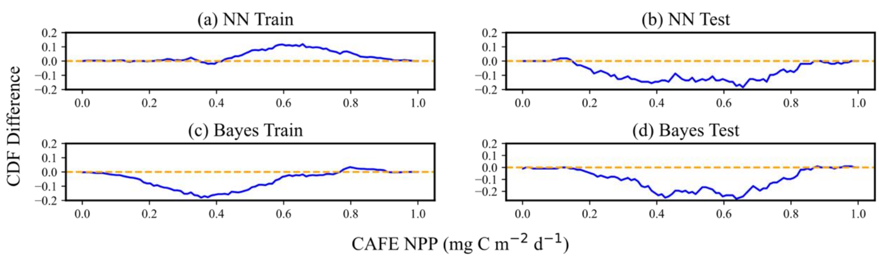

Fig. 9. Difference between the input data CDF and mean CDF of model predictions. Panels (a) and (b) represent the performance of the training set and test sets, respectively, in the neural network-based probabilistic prediction model. Panels (c) and (d) showcase the performances of the training set and test sets, respectively, in the empirical distribution-based Bayesian probabilistic prediction model. The blue curves in each panel indicate the differential magnitude of the CDFs. Instances where the blue curves align with the yellow lines denote zero discrepancy between the input data CDF and the model's predicted mean CDF.

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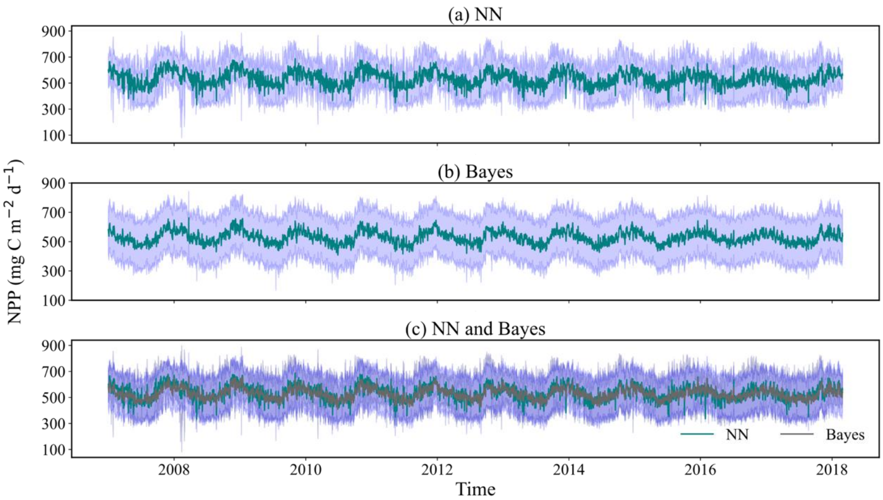

Fig. 10. Time series plots of daily probabilistic NPP predictions in Weizhou Island (2007 – March 2018). (a) Probability prediction results of the neural network model; (b) Bayesian probability prediction results based on empirical distribution; (c) Comparison of the two models' predictions, with the green lines representing the mean predictions from the neural network model and the gray lines depicting the mean predictions from the Bayesian model.

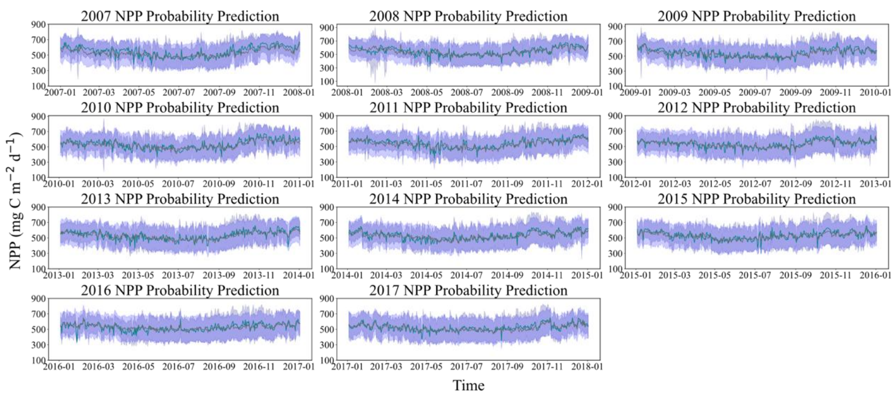

Fig. 11. Time series plots of probabilistic NPP predictions in Weizhou Island (2007 – 2017). The light purple shading indicates the 95% confidence interval of the Bayesian model, while the dark purple shading represents the 95% confidence interval of the neural network model. The green lines show the mean prediction values from the neural network model; and the gray lines depict the mean prediction values from the Bayesian model.