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Spatial heterogeneity of long-range dependence and self-similarity of global sea surface chlorophyll concentration with their environmental impact factors analysis

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Understanding the long-range dependence and self-similarity of global sea surface chlorophyll concentration (SSCC) will enrich its characteristics description and analysis with global change patterns. The satellite SSCC products were collected from the European Space Agency during the period from 29 July 1998 to 31 December 2020. After resampling the SSCC products into the spatial resolution of 1°, the missing values were interpolated by Bayesian maximum entropy with mean absolute error of cross validation equaling to 0.1295 mg/m³. Generalized Cauchy model was employed to quantitatively determine the long-range dependence and self-similarity of SSCC at a global scale by using the Hurst parameter and fractal dimension. Good fitted results were achieved with an averaged R² of 0.9141 and a standard deviation of 0.0518 across the 32,281 spatial locations of the entire ocean; the averaged values of Hurst parameter and fractal dimension were 0.8667 and 1.2506, respectively, suggesting strong long-range dependence and weak selfsimilarity of SSCC in the entire oceans. Univariate and multivariate generalized addictive models (GAM) were introduced to depict the influence of sea surface height anomaly, sea surface salinity, sea surface temperature and sea surface wind on the Hurst parameter and fractal dimension of SSCC; and smaller mean absolute error were achieved for the GAM of Hurst parameter than that of fractal dimension. Sea surface height anomaly showed the strongest influence for the Hurst parameter than the other three factors, and sea surface wind depicted similar influence; the sea surface temperature owned opposite influence on Hurst parameter compared to sea surface salinity.

KEYWORDS

sea surface chlorophyll, long-range dependence, self-similarity, generalized cauchy model, bayesian maximum entropy, generalized addictive model

1 Introduction

Phytoplankton serves as the fundamental source of primary production in the world's oceans. Sea surface chlorophyll concentration (SSCC) is commonly considered as the indicator of the phytoplankton biomass, and was used for primary production estimation [1–3]. It makes a certain contribution to the particulate organic carbon in water and organic matter in sea fog aerosols [4,5]. Studies have shown that phytoplankton, with the highest carbon sequestration capacity in marine ecosystems, can capture 360 billion tons of CO_2 annually, of which 1.39% of CO_2 will be transported to the seabed and stored long-term through the biological pump [6,7]. Understanding the spatial and temporal variation characteristics of SSCC can help estimate the amount of carbon captured in the sea area, clarify the mechanism of marine carbon cycling, and provide scientific bases for algal bloom warning and ocean management.

Based on the autocorrelation characteristics of SSCC, previous studies have developed various time series prediction models, such as long short-term memory neural networks, spatiotemporal attention networks, and hierarchical attention networks [8-10]. When the autocorrelation of SSCC is very strong, it can be considered as long-range dependence. The Hurst exponent is generally used to quantitatively describe the degree of long-range dependence. The generalized fractional Gaussian noise model, generalized Cauchy model, and covariance and variance functions were normally used to calculate the global Hurst exponent [11-13]. Regarding SSCC, the generalized Cauchy model has been utilized to describe the long-range dependence of SSCC at limited number of spatial locations, as well as the selfsimilarity [14,15]. Although the long-range dependence and selfsimilarity of SSCC, respectively, show strong and weak characteristics in the above two literatures, it is essential to explore other locations in the oceans for a more comprehensive deduction. A global-scale investigation of the spatial pattern of these two features (i.e., long-range dependence and self-similarity) will not only provide insights into the spatiotemporal variability of SSCC across a broader area but also offer a mathematical perspective to inform ocean management and ecology. Therefore, such an inquiry would lay a solid foundation for the scientific understanding of SSCC, ultimately aiding in the sustainable management of ocean resources.

Remote sensing technology has been a popular tool to monitoring the SSCC variation in large space-time domain. However, the remote sensing data may have some degrees of data missing, so it becomes an important scientific issue to scientifically analyze and accurately interpolate the data using limited data as much as possible. Previous studies have tested five methods, containing of nearest neighbor, bilinear, smooth filter, sharpening filter, and unsharp masking, for interpolation purposes, and the results indicated that these methods had good interpolation accuracy for high-resolution remote sensing images [16]. However, as early as 1994, Rossi et al. [17] pointed out that nearest neighbor or bilinear interpolation cannot fully utilize the spatial information contained in remote sensing data, and indicated that the Kriging method can overcome this deficiency and applied the indicator Kriging in land classification. Considering the advantages of geostatistical methods in interpolation, the family of Kriging and inverse distance weighting method were compared for water quality evaluation, and the results showed that Kriging outperform IDW [18,19]. Although the spatiotemporal Kriging technology has been developed to include temporal information for spatiotemporal interpolation purposes and more accurate prediction will be achieved than the standard Kriging, it still cannot deal with the non-Gaussian distributed or uncertain data with including high order moments [20-23]. The Bayesian maximum entropy method (BME) is currently the most complete and capable interpolation method in the field of spatiotemporal geostatistics by borrowing the strength from the Bayes theory and maximum entropy theory, and it has been widely used in the fields of environmental science, remote sensing, marine science, public health, etc. [24-29]. Although the BME has been employed to assimilate the information from auxiliary variable and machine learning evaluation for improving the spatiotemporal coverage, accuracy and reducing the uncertainty of remote sensing SSCC product [15,30], there is still a lack of direct application of this method to the interpolation of SSCC over a wider range.

SSCC has a direct or indirect response relationship with environmental factors such as sea surface salinity, temperature, wind speed, etc. [31,32]. Specifically, the high correlation between sea surface salinity and nutrient concentration leads to a certain association between the spatial distribution of SSCC and the salinity front [33,34]. A positive correlation between SSCC and sea surface wind speed was found in the east coastal area of Vietnam [35]. Sea surface wind can also affect the vertical stratification and turbulent mixing of seawater by changing the sea surface temperature, and bring nutrients from the bottom of the sea to the sea surface, such as the Ekman suction effect caused by vortex phenomena, which in turn affects the changes and distribution of sea surface chlorophyll [36,37]. Sea surface temperature exhibits close relationship with SSCC, however, the effects of temperature on SSCC may vary at various regions of ocean [15,28,38]. Therefore, it is worthy to explore the environmental impacts on SSCC in a local scale way.

In view of the above considerations, the main objectives of the current study are threefold: to assess the performance of BME in SSCC interpolation, to quantify the long-range dependence and self-similarity of SSCC at a global scale, and to determine the significance of various environmental factors on the SSCC variation.

2 Materials and methods

2.1 Remote sensing data

The remote sensing SSCC data used in this study was obtained from the European Space Agency (ESA) during the period from 29 July 1998 to 31 December2020. The data is a fusion product based on multiple sensors, including Sea-Viewing Wide Field of View Sensor (SeaWiFS), Medium Resolution Imaging Spectrometer (MERIS), Aqua-Moderate Resolution Imaging Spectroradiometer (MODIS), Visible and Infrared Imager/Radiometer Suite (VIIRS), and Ocean and Land Color Instrument (OLCI), with a spatial resolution of 4 km and a temporal resolution of 1 day. To ensure consistency and facilitate analysis with other environmental factors, the original SSCC data was resampled to a product with a spatial resolution of 1° by averaging the SSCC values within each 1degree grid. In addition, four environmental factors, including sea surface height anomaly, sea surface salinity, sea surface temperature and wind speed, were regarded as SSCC-related variables. Among them, sea surface height anomaly data was downloaded from Copernicus marine service website, and its spatial and temporal resolution is 0.25° and 1 day, respectively; salinity data were also achieved from Copernicus marine service website, and the spatial and temporal resolutions are 0.25° and 1 week; daily sea surface temperature data were obtained from NOAA optimal interpolated SST with spatial and temporal resolutions of 0.25° and 1 day; wind speed data were achieved by the NOAA NCEI blended Seawinds (NBS v2) with spatial and temporal resolutions of 0.25° and 1 day. The sea surface temperature and wind speed data were resampled to the same

2.2 Bayesian maximum entropy modeling and spatiotemporal SSCC interpolation

resolutions of salinity data.

In order to improve the spatiotemporal coverage of remote sensing SSCC data, the BME theory of geostatistics was introduced to absorb the spatiotemporal distribution pattern of SSCC for interpolation purposes. Generally, the spatiotemporal random field (STRF), X(p), was used to describe the spatiotemporal variation of SSCC, where p = (s, t) represents the space-time location, while $s = (s_1, s_2)$ depict the geographical coordinates. To perform spatiotemporal SSCC interpolation, BME absorbs two kinds of knowledge bases (KBs): (a) core or general (G) KB that capturing the space-time SSCC mean trend function $m_X(\mathbf{p}) = \overline{X(\mathbf{p})}$, and the space-time covariance function $c_X(\boldsymbol{p}, \boldsymbol{p}') = \overline{[X(\boldsymbol{p}) - m_X(\boldsymbol{p})][X(\boldsymbol{p}') - m_X(\boldsymbol{p}')]};$ and (b) sitespecific (S) KB including remote sensing SSCC data in the current study. Given both G- and S-KBs into consideration, the probability density functions (PDF) of the possible SSCC values at unmonitored space-time point p_k can be calculated by Eq. (1):

$$f_{K}(\boldsymbol{\chi}_{k}) = A^{-1} \int d\boldsymbol{\chi}_{h} f_{G}(\boldsymbol{\chi}_{h})$$
(1)

Where χ_h and χ_k denote the SSCC values at point p_h and p_k , respectively; f_G and f_K denote the prior space-time PDF obtained from G-KB and the posterior PDF at each unmonitored point p_k , respectively; and A is the normalization constant. More detailed can be found in the relevant literatures [39,40]. In the BME interpolation process, a spatiotemporal moving searching radius was set by centering at the estimation point; specifically, the spatial and temporal radius was 8° and 1 day, respectively. Within the spatiotemporal radius, the up to 12 hard data near the estimation point were employed for generating prior probability density functions. During this procedure, the space-time distance between points were compared by setting the S/T ratio as 1, i.e., the distance of 1° in spatial dimension is equal to the distance of 1 day in temporal dimension. Further, the expected value of the posterior PDF was regarded as the interpolated SSCC values. Leave-one-out cross validation technique was implemented for testing the performance of BME in SSCC interpolation, and the mean absolute error (MAE) and root mean squared error (RMSE) were treated as two indicators for quantifying the accuracy of BME interpolated results.

To further corroborate the accuracy of the BME-interpolated SSCC product, an additional daily gap-free SSCC product employing a modified Data Interpolation Empirical Orthogonal Function (DINEOF) interpolation methodology was procured from the Copernicus website (https://data.marine.copernicus.eu/product/OCEANCOLOUR_GLO_BGC_L4_MY_009_104/

description) for comparative analysis. Subsequently referred to as the GlobColour product, it was resampled from a 4 km resolution to a 1-degree resolution through averaging. Additionally, *in-situ* observations of SSCC data, monitored by Argo buoys, were acquired from https://dataselection.euro-argo.eu/to serve as a validation dataset.

2.3 Modeling the long-range dependence and self-similarity of SSCC by generalized cauchy model

The variant generalized Cauchy model depicted in Eq. (2) comprises two parameters, i.e., Hurst exponent H and fractal dimension D, which are considered as quantitative expressions for long-range dependence and self-similarity of a given time series. If 0.5 < H < 1, it represents long-range dependence with a larger value of H implying a greater dependence of the SSCC series; conversely, if 0 < H < 0.5, it indicates short-range dependence; if H = 0.5, the SSCC time series exhibits white noise characteristics. On the other hand, the values of D range from 1 to 2, with a larger value of D indicating a stronger self-similarity of SSCC series. More detailed information of the formula derivation and proven process can be found in previous studies [13,41].

$$C(\tau) = \left(1 + |\tau|^{4-2D}\right)^{-\frac{1-H}{2-D}}$$
(2)

The model will be fitted to the empirical autocorrelation functions of the considered SSCC time series at various spatial locations with spatial resolution of 1° across the oceans. Further, BME and hotspot analysis were employed for the two parameters (Hurst exponent and fractal dimension) mapping purposes.

2.4 Generalized additive model

In order to explore the significant impact factors, generalized additive model (GAM) were employed for constructing non-linear system between environmental factors and Hurst parameter and fractal dimension of sea surface chlorophyll, as the following equation shows.

$$y_j = a_j + \sum_{i=1}^4 f_i(x_i) + \varepsilon$$
(3)

where x_i represent the environmental variables, i = 1, 2, 3, 4, including sea surface height anomaly, sea surface salinity, sea surface temperature, and sea surface wind; f_i represents the corresponding smoothing spline functions; a_j represents the overall average intercept for Hurst parameter and fractal dimension, j = 1, 2; ε represents the residual; y_j represents the Hurst parameter and fractal dimension. "LinearGAM" function



from the pygam library was employed to process the generalized additive modeling. The parameter "n_splines" is defined to determine the number of splines used for each feature, where each spline corresponds to a small interval. In the current study, the "n_splines" parameter was set to 20. Natural cubic splines were defautly used for fitting within each interval. Consequently, the polynomial order within each interval is typically set to three. Specifically, each cubic spline within an interval is determined by four control points, providing four degrees of freedom. These degrees of freedom determine the coefficients of the cubic polynomial, thereby defining the polynomial function within each interval.

3 Results

3.1 Cross-validation and improvement of SSCC's coverage

Using leave-one-out cross-validation, BME method was validated by the remote sensing chlorophyll concentration data during an 8192-day period. By comparing the BME predicted SSCC values with the remote sensing original values, the results showed that the BME has good capabilities in spatiotemporal

prediction of sea surface estimation and chlorophyll concentration, with MAE and RMSE of 0.1295 mg/m3 and 0.4465 mg/m³, respectively. Then, the BME method was further employed for spatiotemporal SSCC interpolation at 43,337 spatial locations in the global ocean during the entire study period. The numbers of SSCC data for each spatial point before and after BME interpolation are shown in Supplementary Appendix A1A, B of the Appendix Section. respectively. The statistical results showed that each spatial point had an average number of 3,623 data before BME interpolation (covering 44.23% of the study period), while the number increased to 7,351 after BME interpolation (covering 89.73% of the study period). Therefore, the BME method significantly improved the spatiotemporal coverage of remote sensing SSCC data set. The daily averaged SSCC values of the BME-generated product are illustrated in Supplementary Appendix A2A, displaying a distribution pattern akin to the resampled averaged SSCC values of the GlobColour product, as depicted in Supplementary Appendix A2B.

To quantify the disparities between the daily BME-generated SSCC product and the GlobColour product, both MAE and RMSE were calculated, resulting in values of 0.15 and 0.63 mg/m³, respectively. Furthermore, to assess the accuracy of these products, Argo *in-situ* observations were employed for validation. The results revealed MAE and RMSE values of 0.20 *versus* 0.27 mg/



m³ and 0.46 *versus* 0.79 mg/m³, respectively. The corresponding high-density scatter plots are presented in Supplementary Appendix A3.

3.2 Complexity and hot spots of global SSCC

Among the 43,337 spatial points in global oceans, data from 32,281 to 30,926 points respectively have temporal coverage of over 80% and 90% throughout the entire study period. A generalized Cauchy model was used to fit the autocorrelation function of 32,281 time series of SSCC in the global oceans. The statistical results showed that the coefficient of determination (R²) between the fitted values and empirical values of the linear regression equation fluctuated between 0.6610 and 0.9994, with a mean of 0.9141 and a standard deviation of 0.0518. The MAE fluctuated between 0.0029 and 0.2058 mg/m³, with an average value of 0.0387 mg/m³ and a standard deviation value of 0.0227 mg/m³. The RMSE fluctuated between 0.0039 and 0.2304 mg/m³, with an average value of 0.0454 mg/m³ and a standard deviation value of uter a standard deviation value of 0.0257 mg/m³. Figure 1 shows the autocorrelation function (ACF) of nine randomly selected time

series of SSCC from the 32,281 points and the fitting curve of the generalized Cauchy model. It can be seen from the figure that the generalized Cauchy model performs good in modeling the ACF of SSCC. In general, the Hurst exponent (H) of SSCC fluctuated between 0.5 and 0.9632, with an average value of 0.8667 and a standard deviation value of 0.0582. The fractal dimension (D) fluctuated between 1 and 1.9484, with an average value of 1.2506 and a standard deviation value of 0.2459. The spatial locations of the nine selected SSCC time series are presented in Supplementary Appendix A4.

Further, the fractal dimension and Hurst exponent, characterizing the self-similarity and long-term correlation characteristics of SSCC, were mapped by BME, shown in Figure 2. Figure 2A shows that high fractal dimension values are widely distributed in coastal areas of all continents, tropical areas of the North Pacific (except the areas near the equator), the areas of the South Pacific between 0 and 30 degrees, areas near 45 degrees in the South Pacific, areas between 15 and 25 degrees in the North Atlantic, and some regions of the Indian Ocean. Figure 2B shows that high Hurst exponent values are distributed around 30 degrees north and south latitudes in a belt-like pattern. The hot spot analysis made a step ahead for identifying high and low values aggregation areas of



fractal dimension and Hurst exponent in a spatial distribution view, and the results are shown in Figure 3.

3.3 Contributions of four sea surface parameters on hurst parameter and fractal dimension of SSCC

Although all environmental factors, i.e., sea surface height, sea surface salinity, sea surface temperature, sea surface wind, showed statistically significant with p values smaller than 0.001 in both univariate and multivariate GAM, the R square values of the univariate GAM are smaller than 0.2 and the R square values of multivariate GAM are *vice versa*. Regarding the generalized cross validation, the evaluation error of the univariate or multivariate GAM for modeling fractal dimension ranged from 0.0475 to 0.0584, while the corresponding error for modeling Hurst parameter ranged from 0.003 to 0.0034. The results of multivariate GAM and univariate GAM were presented in Figures 4, 5 and Appendix section, respectively. For fractal dimension of sea surface chlorophyll, the impacts of sea surface temperature and sea surface wind showed an overall increasing and decreasing trend,

respectively; the impacts of sea surface height and sea surface salinity depicted an increasing-decreasing and fluctuating trend, respectively. Regarding the Hurst parameter of sea surface chlorophyll, the opposite trends of sea surface temperature and salinity impacts were detected; and similar decreasing-increasingstable trends were found for the impacts of sea surface height and sea surface wind.

4 Discussion

Compared with the Argo *in-situ* SSCC observations, the BMEgenerated SSCC product depicted more accuracy than the GlobColour product, indicating that the BME shows better performance than the DINEOF in SSCC interpolation. On the other hand, compared with the global SSCC distribution shown in the literatures [42,43], as well as the GlobColour product, the BME-generated SSCC product displays similar characteristics, including high- or low-values regions.

The spatial distributions of self-similarity and long-range correlation characteristics of global SSCC were explored for the first time in the current study. Generally, geostatistical



methods are applicable to spatiotemporal analysis of natural attributes with strong spatiotemporal correlation [39,40,44]. This study found that BME will give high accurate prediction for SSCC, indicating that the SSCC may own strong spatiotemporal correlation, which is in line with Tobler's First Law (the first law of geography): everything is related to everything else, but near things are more related than distant things [45]. Similar findings have been confirmed in many studies [15,28,30]. The outcome of this study is that the self-similarity and long-range dependence of SSCC have spatial correlation characteristics, varying in different regions. According to Figures 2, 3, the self-similarity and long-range dependence of SSCC are independent with each other, and their high- and lowvalue distributions are also inconsistent. On one hand, inland human activities often result in high nutrient burden along the coast forming eutrophic regions [43], which promotes algal growth and increase SSCC [46,47]; and it may be one of the reasons for the strong self-similarity characteristics of SSCC. Regarding the high fractal dimension values in the east coastal of United States, it was found that the river discharge from inland will have strong impacts on the circulation, salinity and water quality of the coastal regions of the New Jersey, Cape Hatteras and Florida, further influencing SSCC variations [48,49]. On the other hand, the Hurst exponent distribution indicating the strength of long-range dependence shows a similar distribution pattern to the values of SSCC [28], which suggests that areas with lower chlorophyll concentration or less nutrientrich regions have more stable algal growth and relatively stable changes in SSCC, leading to stronger long-range dependence. For

example, low primary production regions, oligotrophic regions, or the distribution of the depth of the 0.2 mm (ZNO₃) nitrate concentration showed similarities with the hot spots of Hurst parameter in the Pacific Ocean, Atlantic Ocean and Indian Ocean [43,50,51], as the mid-latitude regions (around 30°) in both hemispheres shown in Figure 3B. Moreover, the association between SSCC and sea surface temperature were also strong in these regions, while the distinct boundary located at around 45° latitude, which is due to the switch from negative to positive responses of SSCC to marine heatwaves [28,52].

Given the relatively weak self-similarity of SSCC, this discussion focuses solely on the long-range dependence of SSCC. The growth of phytoplankton is a continuous process that is influenced by environmental factors, such as nutrient concentration. The multivariate GAM results indicate that among the four factors, the sea surface height anomaly has the greatest influence on the long-range dependence of SSCC, as represented by the Hurst parameter (Figure 5). The sea surface height anomaly is associated with anticyclone- and cyclonerelated eddies, which can transport nutrients from deeper sea layers to the surface, promoting phytoplankton growth [53-56]. The curve shown in Figure 5A demonstrates that cyclone-related eddies have a positive influence on the Hurst parameter, while anticyclone-related eddies have a negative influence. The contrasting impacts of sea surface temperature and salinity on the long-range dependence of SSCC, as shown in Figures 5B,C, result from the varying responses of different phytoplankton species or communities [57-61]. In other words, specific temperature and salinity conditions favor certain species or



communities of phytoplankton, leading to their dominance and higher long-range dependence. Sea surface wind enhances mixing between surface and deeper waters, consequently impacting nutrient levels. Low wind speeds maintain favorable conditions for phytoplankton growth and keep SSCC at a relatively stable level. Strong winds with appropriate direction relative to the coast and hemisphere also contribute significantly to coastal upwelling, facilitating nutrient transport [35,62], thereby resulting in the high long-range dependence of SSCC observed in Figure 5D.

As the present study exclusively delved into examining the monofractal and long-range dependence characteristics of SSCC, future investigations could pivot towards the detection and quantification of multifractal features within SSCC, drawing inspiration from previous works [63–65]. Concurrently, an avenue for further exploration lies in dissecting the seasonal aspects of the long-range dependence and selfsimilarities inherent in SSCC, providing an opportunity for more comprehensive insights in future research. It should be acknowledged that the BME-generated SSCC at the north region of Russia may include uncertainty due to lack of remote sensing data (Supplementary Appendix A1, A2). Therefore, it is also worthy to find proper ways to improve the BME products at the polar regions in the future.

5 Conclusion

In the current study, the performance of BME on SSCC interpolation was evaluated as robust and effective with mean

absolute error of cross validation equaling to 0.1295 mg/m³. The temporal variations of SSCC across the entire oceans were described using the generalized Cauchy model, and good performance was obtained with mean value of the R² equaling to 0.9141. The findings revealed strong long-range dependence and relatively weak selfsimilarity of SSCC; specifically, the values of Hurst parameter and fractal dimension ranged from 0.5 to 0.9632 and from 1 to 1.9484 with the mean values of 0.8667 and 1.2506, respectively. Further, the midlatitude regions exhibited the highest long-range dependence, while the coastal regions showed the greatest self-similarity of SSCC. The use of GAM revealed that both sea surface height anomaly and sea surface wind made similar contributions to the long-range dependence of SSCC. Conversely, sea surface temperature and sea surface salinity had opposite effects on the long-range dependence of SSCC. Sea surface temperature is always positively correlated with the long-range dependence of SSCC.

Data availability statement

The original contributions presented in the study are included in the article/Supplementary Material, further inquiries can be directed to the corresponding author.

Author contributions

JH: Conceptualization, Formal Analysis, Funding acquisition, Methodology, Validation, Visualization, Writing-original draft, Writing-review and editing. ZG: Formal Analysis, Investigation, Methodology, Validation, Visualization, Writing-review and editing. YJ: Formal Analysis, Investigation, Methodology, Validation, Visualization, Writing-review and editing. ML: Conceptualization, Methodology, Resources, Writing-review and editing.

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Supplementary material

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fphy.2024.1331660/ full#supplementary-material

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