Improved Perceptron of Subsurface Chlorophyll Maxima by a Deep Neural Network: A case study with BGC-Argo float data in the northwestern Pacific Ocean

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1. Aim

In this study, we develop a deep neural network (DNN) model to retrieve the vertical profiles of Chl *a* from surface-ocean data which are equivalent to the average value within the first 20 m water depth. Our DNN model has at least 3 hidden layers in the algorithm. Compared to the shallow ANN, such an improvement theoretically helps to improve performance for prediction capability. Rather than using the sigmoid activation function, we use a Gaussian radial basis activation function in the DNN model, which is one of the most frequently used radial functions in the literature. We train the DNN model by inputting sea surface temperature (SST) and surface Chl *a* from Biogeochemical-Argo (BGC-Argo) floats. We apply the DNN model to the northwestern Pacific Ocean and compare the estimated vertical Chl *a* profiles and associated SCM characteristics with observations in different regions and seasons. Finally, we examine the prediction capability of our DNN model in retrieving vertical Chl *a* profiles from remote-sensing data in the northwestern Pacific Ocean.

2. Procedure

2.1 Improved DNN model

The DNN model is an extension of a conventional ANN, with at least two hidden layers between the input and output layers. Because each node in the hidden layer makes both associations and grades of the input to determine the output, stacking more of these layers upon each other benefits more from multiple hidden layers (Figure 1). After processing the signals by the neurons in the hidden layer, the DNN passes them to the output layer. Then, by comparing and calculating the output error with the target, backward propagation is used to adjust the weight of signals in the hidden layers and further reduce the error using the optimisation algorithm.

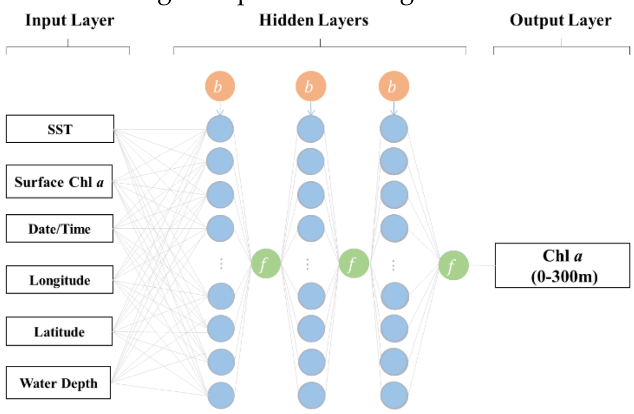

Figure 1. Structure of the deep neural network (DNN). The input elements of DNN are longitude, latitude, time, sea surface temperature (SST), sea surface Chl *a*, water depth. The output is the vertical distribution of Chl *a* concentration over the water depth of 0–300 m. *b* is the bias term in the hidden layer. The prior information of nonlinear activation function (*f*) connects the hidden layers to the output.

In the calculation of SCM characteristics, we improved the existing DNN model in the following two aspects. First, we improve the capability of model for the calculation of SCM depth by replaced the bias term b (that is, the intercept term) from random values to annual mean of SCM depths (Equation 1).

$$b_{SCM} = \frac{avg(z_{\max})}{\max(z)}, \tag{1}$$

where z is the water depth, max(*z*) is set to 300 m by assuming that there is no Chl *a* below 300 m depth, and $avg(z_{\max})$ is the annual mean of SCM depth ($z_{\max}$).

In the second aspect, we improve the calculation accuracy of model for the SCM intensity and thickness. Considering the unimodal chlorophyll profiles, a Gaussian radial basis function is substituted for the sigmoid function as a nonlinear activation function (*f*, Equation 2) in the original DNN model to amplify the signals within the SCM layer.

The advantage of Gaussian radial basis activation function is that it is similar to quadratic function for the center values of input variables, while the sigmoid activation function is similar to linear function about the moderate inputs.

$$f = e^{-\pi(X_j - b_{SCM})^2}, \quad (2)$$

where X_j is the X value of the j^{th} output in the hidden layer, and b_{SCM} is the bias term computed by the annual mean of SCM depth (Equation 1). The Gaussian radial basis activation function helps to absorb the information of the annually averaged SCM depth and, hence, further extract the SCM features.

Consequently, a DNN model with at least 2 hidden layers was applied due to its availability in capturing the nonlinear relationships, and the annual averaged SCM depth is incorporated into both the bias term and the Gaussian radial basis activation function to improve the capability in retrieving the SCM characteristics. We name this improved model as IDNN model.

2.2 BGC-Argo Data for the IDNN Model

The in situ data for the IDNN model were collected from 16 BGC-Argo profiling floats in the northwestern Pacific Ocean (https://biogeochemical-argo.org/). Figure 2 plotted the trajectories of the 14 BGC-Argo profiling floats within 123 °E–180 °E, 12 °N–48 °N, where a SCM feature was observed. Figure A1 showed the locations of vertical Chl *a* profiles observed from 16 BGC-Argo floats in the absence of a SCM. The acquired 2409 vertical Chl *a* profiles, covering four seasons during the period from July 2017 to April 2021, were used in our study after quality control to remove aberrant data caused by electronic noise.

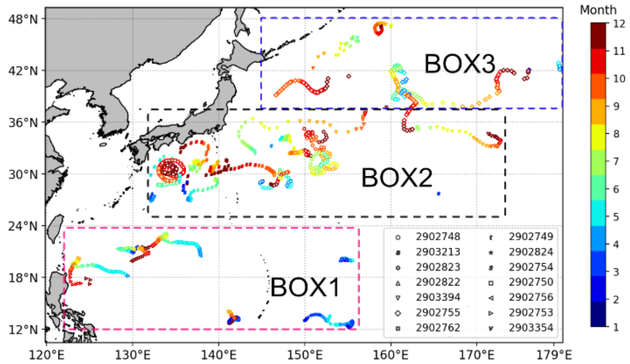

Figure 2. Locations and measuring months of 14 BGC-Argo profiles with a subsurface chlorophyll maximum (SCM) feature in the northwestern Pacific Ocean.

Most vertical profiles of Chl *a* showed a unimodal distribution, while the remaining minors showed either increasing or decreasing Chl *a* with depth. Here, focusing on the SCM patterns, we structure each BGC-Argo vertical profile based on a Gaussian function assumption (Equation 3).

$$Chl(z) = Ae^{-\frac{(z - z_{\max})^2}{2\sigma^2}}, \quad (3)$$

where σ is its standard deviation, A is the amplitude of the Gaussian curve, and $z_{\max}$ is the location of the amplitude. To quantify the vertical scale of the SCM layer, 2σ was used to represent the SCM thickness. Because the upper layer of the SCM ($z_{\max} - \sigma$) must be inside the water, it is set as a nonnegative value. That is, if $z_{\max} - \sigma < 0$, the upper layer of the SCM is set to the sea surface (0 m). In addition, the SCM intensity refers to the peak value of Chl *a* concentration (A).

The values of the Gaussian parameters (σ, A and $z_{\max}$) were obtained by fitting all observed vertical Chl *a* profiles, which can be used to filter out Chl *a* profiles with no significant SCM characteristics via the following three steps. First, profiles with the values of parameter σ ranging from the lower limit of the data value to half of the upper limit (0–48 m), are kept, thereby leaving 1676 profiles. Second, parameter A (the peak values of Chl *a* obtained from Gaussian fitting) was assumed to be at least twice the surface Chl *a* concentrations. Meanwhile, values larger than the upper limit (2.2 mg m^{-3}) were neglected as outliers. This step excluded 328 profiles. Third, z_{max} values are limited to depths above 200 m. Finally, after visually reviewing all the filtered profiles, 1342 out of the total 2409 profiles were retained in the following analysis. Consequently, the remaining vertical Chl *a* profiles present a significant SCM characteristics.

2.3 Satellite Data for the IDNN Model

To evaluate the performance of IDNN reconstruction using remote-sensing data, the MODIS Level 3 standard mapped image monthly Chl *a* and SST database with a 9 km spatial resolution were downloaded (http://apdrc.soest.hawaii.edu/dods/public_data/satellite_product/MODIS_Aqua/) and used to extract the input values for the IDNN model.

2.4 Training Process

In our IDNN model, SST, sea surface Chl *a*, associated geo-location (latitude, longitude) and observation time, and water depth were selected as input variables (Figure 1), which are similar to the study by Sammartino *et al.*

The IDNN model was trained in each BOX, respectively. 75% of the input data and vertical profiles of Chl *a* from BGC-Argo floats in each BOX were segmented and fed into the IDNN model as the training set, which was selected randomly. During the training process, 15% of the training set was randomly selected as a validation set to verify whether the IDNN model was over-fitted. According to the performance of the validation set, the parameters of the IDNN model were determined using a grid search.

To evaluate the errors between the IDNN output and the observed value, the determination coefficient (R^2), correlation coefficient (ρ), root mean square error (RMSE), mean absolute percentage error (MAPE), and mean bias error (MBE) are introduced as cost functions. The R^2 and RMSE values were used as performance indicators to evaluate the effectiveness of the developed models. MAPE and MBE capture the average difference between the estimated and observed values.

3 Results and Discussion

3.1 IDNN-retrieved Chl a Vertical Profiles

After evaluating the IDNN performance on a training set, we applied the IDNN model to a test set. Here, the test set contains 25% of the total BGC-Argo surface Chl *a* and SST datasets. In the testing phase of the IDNN model, a trained network was used for forward estimation. The data on the test set are normalised in a similar manner to that in the training set, with the network output being inversely normalised to the original unit. As shown in Figure 3, the modelled Chl *a* concentrations from the test set are closely comparable with the observed values for the upper 300 m in each BOX.

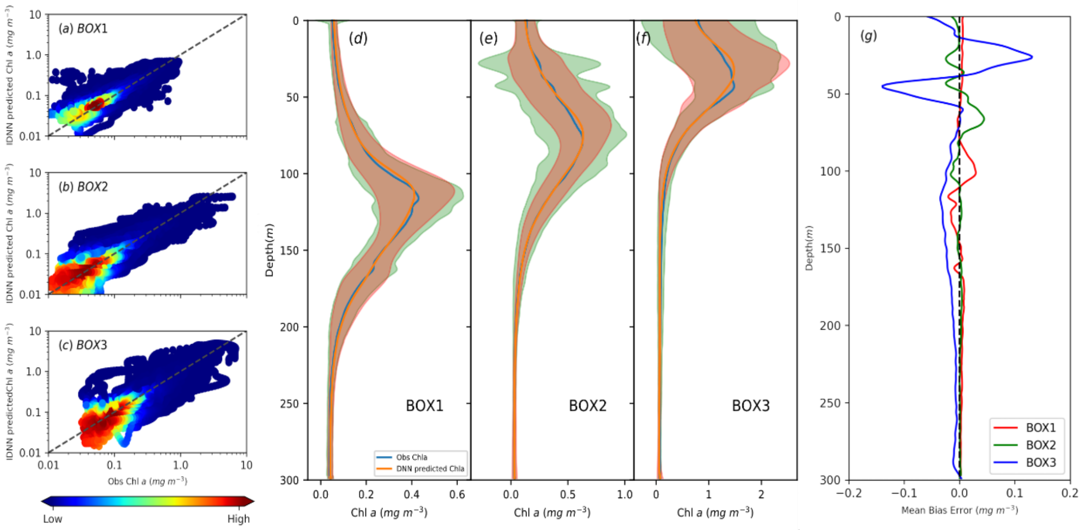

Figure 3. (a–c) Scatter plot of observed Chl *a* concentration (x-axis) and estimated Chl *a* value (y-axis) in BGC-Argo test set in BOXes 1-3. The black dashed line is the bisector of the first quadrant, i.e., y=x. (d–f) The mean of observed value (blue line) and the mean of IDNN predicted values (orange line) in each BOX. The pink and green shades are the standard variance of the model results and observations, respectively, which overlap and form the brown shade. (g) The mean relative bias as a function of the adjusted depth between observed and the IDNN predicted Chl *a* in the test set for the three BOXes. The adjusted depth is defined as the differences between the observed SCM depth and the modeled one.

The statistical indices calculated for the IDNN assessment from the test set are listed in Table 1. The statistical results indicate a robust prediction capability of the IDNN in three BOXes.

Table 1. Statistical results of the comparison between the observed Chl *a* values and the predicted Chl *a* concentration by the IDNN models using BGC-Argo data. R^2 refers to the Determination Coefficient, ρ to the Pearson's Correlation Coefficient, RMSE denotes the Root Mean Square Error, and MAPE represent the Mean Absolute Percentage Error.

Index	Region		
	BOX1	**BOX2**	**BOX3**
R^2	0.77	0.72	0.71
ρ	0.89	0.88	0.87
RMSE	0.0040	0.025	0.11
MAPE	0.036	0.073	0.13

3.2 IDNN-retrieved SCM Characteristics

We apply the IDNN model to calculate the seasonality of SCM characteristics. As shown in Figure 4, the regionally averaged Chl *a* profile predicted by the IDNN model from surface data is comparable to the observations for four seasons.

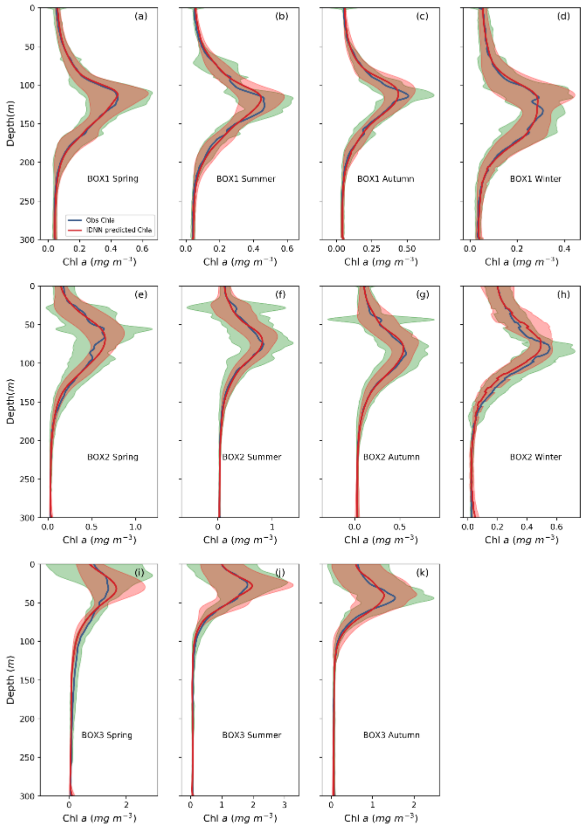

Figure 4. Aggregated chlorophyll vertical profiles from the test set in terms of seasons in BOX1 (a-d), in BOX2 (e-h), and in BOX3 (i-k). The blue and red solid lines represent the mean of observed value and the mean of IDNN predicted Chl *a*, respectively. The pink and green shades are the standard variance of the model results and observations, respectively, which overlap and form the brown shade.

Figure 5 shows that the mean vertical Chl *a* profile inferred by the IDNN from remote-sensing data agrees well with the mean BGC-Argo profile in each BOX, validating the good prediction accuracy of the IDNN model in the northwestern Pacific Ocean.

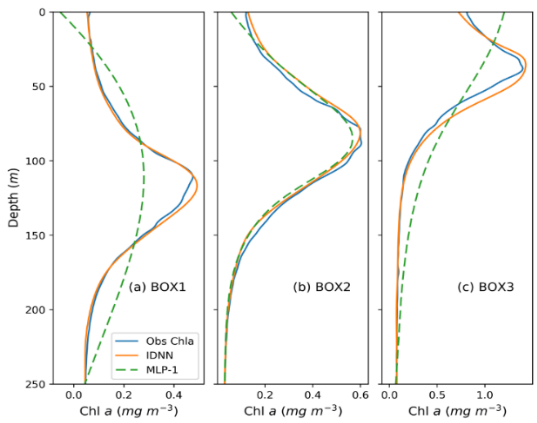

Figure 5. Comparison of the mean profiles of observed values (blue line), IDNN predictions (orange line) and MLP-1 predictions (green dash line) inferred from remote-sensing data in three BOXes.

4 Conclusion

In this study, for the first time, we developed and applied an improved DNN model with Gaussian radial basis activation function, to retrieve the vertical structure of Chl *a* concentration and the associated SCM characteristics in the northwestern Pacific Ocean. The annually averaged SCM depth was incorporated into the bias term and the Gaussian radial basis activation function via the training process of the DNN model, which improved the prediction capability of model from surface-ocean Chl *a* data and SST. The vertical structure of Chl *a* concentration and SCM characteristics, which were estimated by our DNN model, showed a good agreement with observations in different seasons and along the trajectory of BGC-Argo floats. Compared to a series of neural network methods, our IDNN model with Gaussian radial basis activation function captured the SCM characteristics in the northwestern Pacific Ocean, especially in subpolar areas with high surface Chl *a* concentrations. Moreover, the SCM characteristics were reproduced well by our IDNN model inputting remote-sensing surface data.

5 Publication/conference presentation

The article “"Improved Perceptron of Subsurface Chlorophyll Maxima by a Deep Neural Network: A Case Study with BGC-Argo Float Data in the Northwestern Pacific Ocean" ” has been published in *Remote Sensing* **2022**, *14*(3), 632; **https://doi.org/10.3390/rs14030632**

6 Perspectives in the future

This study used surface-ocean Chl *a* and SST as input variables for the IDNN model to reconstruct the non-uniform vertical Chl *a* profiles. A future improvement of our model is to employ additional input variables such as photosynthetically active radiation, light attenuation coefficient, and oceanographic parameters (e.g., sea surface height and wind components) that potentially affect SCM characteristics. Meanwhile, the training process of present IDNN is pixel-to-pixel without considering temporal variations of neighboring pixels, which is similar to other shallow ANN models. Thus, a deep learning technique with a combination of convolution neural network (CNN) and a long short-term memory (LSTM) neural network will be adopted to predict the target by considering the time series of the most correlated surrounding pixels.