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Reconstruction of global surface ocean pCO_2 using region-specific predicators based on a stepwise FFNN regression algorithm

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Abstract: Various machine learning methods were attempted in the global mapping of surface ocean partial pressure of CO_2 (pCO_2) to reduce the uncertainty of global ocean CO_2 sink estimate due to undersampling of pCO_2. In previous researches the predicators of pCO_2 were usually selected empirically based on theoretic drivers of surface ocean pCO_2 and same combination of predictors were applied in all areas unless lack of coverage. However, the differences between the drivers of surface ocean pCO_2 in different regions were not considered. In this work, we combined the stepwise regression algorithm and a Feed Forward Neural Network (FFNN) to selected predicators of pCO_2 based on mean absolute error in each of the 11 biogeochemical provinces defined by Self-Organizing Map (SOM) method. Based on the predicators selected, a monthly global 1° × 1° surface ocean pCO_2 product from January 1992 to August 2019 was constructed. Validation of different combination of predicators based on the SOCAT dataset version 2020 and independent observations from time series stations was carried out. The prediction of pCO_2 based on region-specific predicators selected by the stepwise FFNN algorithm were more precise than that based on predicators from previous researches. Appling of a FFNN size improving algorithm in each province decreased the mean absolute error (MAE) of global estimate to 11.32 μatm and the root mean square error (RMSE) to 17.99 μatm. The script file of the stepwise FFNN algorithm and pCO_2 product are distributed through the Institute of Oceanology of the Chinese Academy of Sciences Marine Science Data Center (IOCAS; http://dx.doi.org/10.12157/iocas.2021.0022, Zhong et al., 2021).

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1 Introduction

As a net sink for atmospheric CO_2, global oceans have been thought to have removed about one third of anthropogenic CO_2 since the beginning of the industrial revolution (Sabine et al., 2004; Friedlingstein et al., 2019). However, great differences existed between previous estimates of sea-air CO_2 flux, due to large uncertainty in estimates of surface ocean partial pressure of CO_2 ($p$$CO_2$) (Regnier et al., 2013; Schuster et al., 2013; Wanninkhof et al., 2013; Ishii et al., 2014). surface ocean $p$$CO_2$ is an essential parameter to describe the release and uptake for atmospheric CO_2 by the oceans in the data-based method. Greater $p$$CO_2$ of surface water than that of overlying air indicating that CO_2 released from oceans to the air, and absorption of CO_2 by oceans happened when the $p$$CO_2$ of surface water was lower than that of air. The ocean in these two scenarios is known as oceanic carbon source and oceanic carbon sink respectively. Sparse and uneven observations of surface ocean $p$$CO_2$ in time and space severely limited the understanding of interannual variability of oceanic carbon sink, and researches based on different methods were carried out to break this barrier. In earlier studies, traditional unitary and multiple regression methods between surface ocean $p$$CO_2$ and its drivers was attempted in the mapping of surface ocean $p$$CO_2$, which were limited in specific regions and sometimes even in specific seasons with a relatively high root mean square error (RMSE) (Sarma et al., 2006; Takahashi et al., 2006; Shadwick et al., 2010; Chen et al., 2011; Marrec et al., 2015). Recent researches on artificial neural networks and other machine learning algorithms, such as feed-forward neural network (FFNN) method (Zeng et al., 2014; Zeng et al., 2015; Moussa et al., 2016; Denvil-Sommer et al., 2019) and self-organization mapping (SOM) method (Friedrich and Oschlies, 2009; Telszewski et al., 2009; Hales et al., 2012; Nakaoka et al., 2013), significantly reduced the bias in the interpolation based on relationships between surface ocean $p$$CO_2$ and its drivers. In addition, method such as finding better predicators or combining SOM and other neural networks was also attempt to further decrease the $p$$CO_2$ predicting error (Hales et al., 2012; Nakaoka et al., 2013; Landschuetzer et al., 2014; Chen et al., 2019; Denvil-Sommer et al., 2019; Zhong et al., 2020; Wang et al., 2021). However, the selection of predicators in the surface ocean $p$$CO_2$ mapping was more empirical, focusing on the theoretical drivers of the $p$$CO_2$ and its variation. Sea surface temperature and salinity were considered as the most important and used in almost all related studies (Landschutzer et al., 2013; Nakaoka et al., 2013; Moussa et al., 2016; Laruelle et al., 2017; Zeng et al., 2017; Denvil-Sommer et al., 2019), similarly the chlorophyll-a concentration is also widely used (Nakaoka et

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al., 2013; Landschuetzer et al., 2014; Laruelle et al., 2017; Zeng et al., 2017; Denvil-Sommer et al., 2019). One more indicator, mixed layer depth, appeared frequently in related studies (Telszewski et al., 2009; Nakaoka et al., 2013; Landschuetzer et al., 2014; Zeng et al., 2017; Denvil-Sommer et al., 2019). Besides, the sampling information have been also used as indicators, including latitude and longitude (Friedrich and Oschlies, 2009; Jo et al., 2012; Zeng et al., 2015; Zeng et al., 2017; Denvil-Sommer et al., 2019), and sampling time (Friedrich and Oschlies, 2009; Zeng et al., 2015). In recent researches, dry air mixing ratio of atmospheric CO_2 (xCO_2) was also used as a predicator (Landschuetzer et al., 2014; Denvil-Sommer et al., 2019). The sea surface height, which was considered effective in improving the spatial pattern and the accuracy of surface ocean $p\mathrm{CO_2}$ mapping at the basin and regional scale, and the monthly anomalies of the most widely used parameters mentioned above were used by the Denvil-Sommer et al (2019). In the research focused on the surface ocean $p\mathrm{CO_2}$ mapping of coastal areas, the bathymetry, sea ice and wind speed were also used as indicators (Laruelle et al., 2017). In each of these researches, same combination of indicators was applied in all areas of the global ocean, although the global ocean was divided into several biogeochemical provinces in some of the researches. However, the indicator that plays an important role in the surface ocean $p\mathrm{CO_2}$ reconstruction at one region may be not a good predicator of surface ocean $p\mathrm{CO_2}$ in other regions, due to complex and variable drivers in different regions. But no widely recognized method for judging the importance of each predicator in the surface ocean $p\mathrm{CO_2}$ mapping are available yet. Thus, we attempted to construct a stepwise FFNN algorithm to rank the importance of predicators and figure out the optimal combination in each biogeochemical province defined by SOM, for decreasing the predication errors in the surface ocean $p\mathrm{CO_2}$ mapping.

2 Methodology

2.1 Data

The surface ocean fugacity of CO_2 ($f\mathrm{CO_2}$) observation data from the Surface Ocean CO_2 Atlas $f\mathrm{CO_2}$ dataset version 2020 (SOCATv2020) (Bakker et al., 2016) was used to construct the non-liner relationship between surface ocean $p\mathrm{CO_2}$ and predicators. The transition between $f\mathrm{CO_2}$ and $p\mathrm{CO_2}$ was following the formula (Körtzinger, 1999):

$$f\mathrm{CO_2} = p\mathrm{CO_2} \cdot exp\left(P \cdot \frac{B+2\delta}{RT}\right) \tag{1}$$

where P is the total atmospheric surface pressure using the National Centers for Environmental Prediction (NCEP) monthly mean sea level pressure product (Dee et al.,

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2011), and T is the absolute temperature. R is the gas constant (8.314 J K^{-1} mol^{-1}). Parameters B and δ are both viral coefficients (Weiss, 1974).

In this work, parts of indicators was choose from previous researches of surface ocean pCO_2 reconstruction based on machine learning methods, including sea surface temperature (SST) and sea surface salinity (SSS) using the 1°×1° gridded product from Chen et al (2017) at http://159.226.119.60/cheng/ and the anomalies (SST_{anom} and SSS_{anom}), chlorophyll-a concentration (CHL-a) and the anomaly (CHL-a $_{anom}$) using satellite derived monthly product in 9 km resolution (Hu et al., 2012), mixed layer depth (MLD) and sea surface height (SSH) and the anomalies (MLD_{anom} and SSH_{anom}) using the ECCO2 cube92 daily product (Menemenlis et al., 2008), W velocity of ocean currents (W_{vel}) at 5, 65, 105 and 195 m depth using the ECCO2 cube92 3-day product (Menemenlis et al., 2008), dry air mixing ratio of atmospheric CO_2 (xCO_2) and the anomaly ($xCO_{2\ anom}$) from the GLOBAL VIEW marine boundary layer product (GLOBALVIEW-CO2, 2011), sea ice area fraction using the monthly product from ECMWF ERA Interim(Dee et al., 2011), 10 meters wind speed using the monthly product from ECMWF ERA Interim (Dee et al., 2011), bathymetry from ETOPO2 (Commerce et al., 2006) , year and month (represented by 1-12), the total number of months since January 1992 (N_{mon}), the sine of latitude and the sine and cosine of longitude (sLat, sLon and cLon). In addition, 8 parameters which were only used in similar previous research focused on other parameters, or were possibly related to the driver of surface ocean pCO_2 and its variability, were selected to be tested. These parameters included nitrate, phosphate, silicate and dissolved oxygen (DO) using the monthly climatology product from WOA18 (Garcia et al., 2019a, b), sea level pressure (SLP) and surface pressure from the ECMWF ERA Interim (Dee et al., 2011), the Oceanic Nino Index (ONI) (Huang et al., 2017), the Southern Hemisphere Annular Mode Index (SAM) (Marshall, G. J., 2003).

2.2 Biogeochemical provinces defined by the Self-Organizing Map

For applying different combination of indicators in regions based on the differences in the dominated drivers of pCO_2 and its variability, the global ocean was divided into a set of biogeochemical provinces using a Self-Organizing Map (SOM) method. The monthly climatology of temperature, salinity, nitrate, phosphate, silicate, and dissolved oxygen were put into a 3-by-4 size SOM networks to generate 12 biogeochemical provinces, where the monthly climatology data in all 12 months were put into one SOM network to generate one discrete set of biogeochemical provinces. Then the discrete small "island" provinces and provinces lack of SOCAT pCO_2 data were merged into the

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nearest dominated province, and the provinces covering areas separated by land were further divided artificially. The final version includes total 11 biogeochemical provinces. In this study the coastal area was not involved and the boundary was defined as 200m depth. In addition, the pCO$_2$ mapping based on SOM defined provinces tend to be less smooth near the border of different biogeochemical provinces, with obvious border line appearing. However, applying of different predictors may make this problem worse. To obtain a smoother distribution, we defined that the grid within 5 1°×1° grids of province borders belong to all provinces adjacent to the nearest province border. Samples in these grids were involved in the FFNN training process of multiple provinces, but only counted once in the validation.

2.3 Stepwise FFNN algorithm

For finding better combination of pCO$_2$ predicators, a stepwise FFNN algorithm was constructed. We used the idea of the multiple linear stepwise regression, replacing the linear regression part by a Feed-forward neural networks (FFNN). The mean absolute error (MAE) difference that before and after adding or removing one indicator in the input of FFNN was used to estimate the performance of each indicator in the FFNN predicating. Although the root mean square error (RMSE) was widely used for the validation of machine learning methods. Compared to the MAE, the RMSE was more sensitive to a few extreme samples, which were generally deviated far from the FFNN predicting values, resulting in a huge discrepancy between the FFNN outputs and pCO$_2$ observations sometimes up to hundreds of μatm. A higher weight may be put on these few extreme samples than other samples in the predicator selection if the performance of each indicator was estimated by RMSE in the stepwise FFNN algorithm. To avoid the higher weight on these few extreme samples, the MAE was used instead in the stepwise FFNN algorithm. The basic principle of the stepwise FFNN algorithm was adding each indicator from a set of indicators into the inputs of FFNN and removing each redundant indicator from the inputs successively to reduce the MAE between the FFNN outputs and SOCAT pCO$_2$ values in the fastest way, until no decrease in the MAE appearing (Fig. 1), where the indicator having no contribution to reduce the prediction error was considered as redundant.

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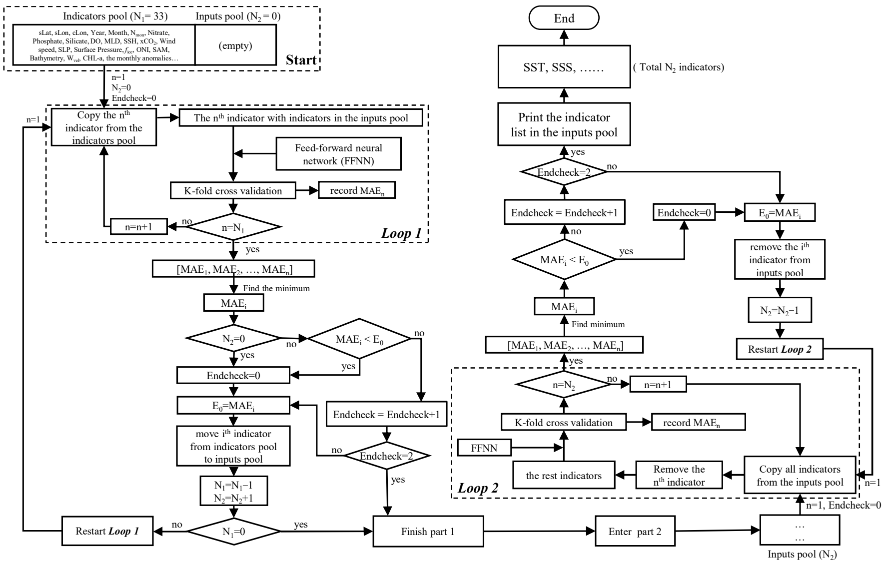

Figure 1. the procedure of stepwise FFNN algorithm

In the beginning of the stepwise FFNN algorithm, all available indicators were put into a matrix, referred to as indicators pool, where each of rows represents one indicator and each of columns represents one SOCAT sample. In this work we collected 33 parameters for test, that is, the indicators pool matrix has 33 rows. Meanwhile a matrix, referred to as inputs pool, was set up to storage indicators with good performance, where good performance means that adding these indicators as predicators can significantly decrease the MAE between SOCAT pCO_2 measurements and FFNN pCO_2 predictions. Then a loop of K-fold validation test run out to calculated the MAE that predicting pCO_2 by each one indicator in the indicators pool in the first step (loop 1 in the Fig. 1). Thus total 33 MAE values were obtained and the minimum was recorded as E_0. The indicator that corresponds to the minimum of all MAE values was moved from the indicators pool to the inputs pool. After that the loop 1 restarted, i.e., the second step started with one indicator removed to the inputs pool and the rest 32 indicators waiting to be tested. Then 32 MAE values of predicting pCO_2 by each one of the rest indicators in the indicators pool with the addition of all indicators in the inputs pool were calculated out. If the MAE in the lowest situation, represented by the MAE_i, decreased compared to the E_0, the i^{th} indicator was considered as a good indicator and was moved from the indicators pool to the inputs pool as well. Then the value of E_0 was replaced by the MAE_i. This part was repeated that the good indicators were selected out in one-by-one step and moved to the inputs pool in the way that the E_0 decreases in the fastest way, until no indicator was left in the indicators pool or no decrease can be found no

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matter which indicator was added in the next two steps. At this time the part 1 of stepwise FFNN algorithm finished, and all indicators left in the indicators pool were considered redundant. The loop K-fold validation in the second part run out in a opposite way that the MAE was calculated with the indicators were removed from the inputs pool one by one in the way that the E_0 decreases the fastest (loop 2 in Fig. 1). The second part was aimed to remove the indicator that can be represented by other indicators in the inputs pool, and finished in the similar condition that no significant decrease can be found no matter which indicator was removed in the next two steps.

The FFNN is composed of four main parts, which are namely input, hidden, summation and output layer (Fig.2). The input layer is designed to pass the inputs to the hidden layer and the number of neurons is equal to the dimensions of the input matrix *p*. The hidden layer includes 25 neurons in the FFNN model, with the tan-sigmoid function as the transfer function. The input *p* is multiplied by a matrix of weights (w_1 in Fig. 2) and the inner product between the result and a bias matrix (b_1 in Fig. 2) is calculated as the input of the transfer function in the first hidden layer. In the summation layer, the transfer function f_2 is a pure linear function. The output of the hidden layer is multiplied by another matrix of weights and summed. All bias and weights matrixes were randomly assigned in the beginning of FFNN training. Here we set one constant random number stream in the MATLAB, thus the way that the bias and weights matrixes randomly assigned were steady, avoiding the appearance of inconsistent results when algorithm repeats.

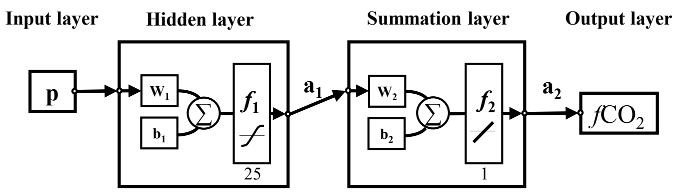

Figure 2. The structure of feed-forward neural network. **p**: input matrix; **w**: weighted matrix; **b**: bias matrix; $\sum$: sum; $\boldsymbol{f_1}$: tan-sigmoid transfer function; $\boldsymbol{f_2}$: pure linear function; **a**: output matrix.

2.4 *p*CO_2 product

Dataset of parameters except CHL-a start since 1992 or earlier, while CHL-a data ranges from 2002 to present. In each one of the provinces, the stepwise FFNN algorithm was run out once first based on all samples covered by CHL-a data, then the algorithm was run out secondly based on samples and all indicators except CHL-a and CHL-a_{anom} in the year that CHL-a gridded data was not available. The *p*CO_2 mapping in the year that CHL-a gridded data was not available was carried out based on the predicators selected in the second run. Although the performance may improve with the number of

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neurons increasing, the influence of number of neurons on the performance of FFNN pCO_2 prediction remains unclear. To further decrease the predicating error between FFNN outputs and SOCAT measurements, the number of neurons was improved by an error test in each province. The number of neurons increased from 10 to 70 and the corresponding MAE values of each size were record, and then the number of neurons with lowest MAE was applied. This test avoided the appearance of insufficient learning capacity for complex nonlinear relationship due to too few neurons and overfitting problem due to too many neurons. Finally, based on the indicators selected by the stepwise FFNN algorithm and improved FFNN size, a monthly global 1°×1° surface ocean pCO_2 product from 1992 to 2019 was constructed.

2.5 Validation

To better estimate the predicating error of FFNN, the MAE and additionally the RMSE which was widely used in previous researches, were calculated using a K-fold cross validation method. To avoid overfitting caused by a lack of independence between the training samples and testing samples, the SOCAT samples were put in chronological order and then divided into group of years (Table 1). In this paper, the value of K was set as 4. Thus, among every 4 neighboring years, three group samples were used for training FFNN model and the rest one was used for testing. Total 4 iterations were carried out, where testing year changed in each iteration. After 4 iterations finished, all samples have been used for testing only once, and the MAE and RMSE between FFNN output and the testing samples was calculated. The performance of the predicator selection algorithm was estimated by comparing the MAE and RMSE result of the FFNN based on stepwise selected indicators with the result based on indicators used in previous researches in each biogeochemical province (Table 2). All validation groups were applied with same FFNN and same samples from SOCAT, with the only differences in predicators. Same K-fold validation procedure was applied for three validation groups based on different pCO_2 predicators. Thus, three results were generated to estimate whether the stepwise FFNN algorithm can effectively find better combination of pCO_2 predictors. Finally the pCO_2 data generated in all validation groups were further compared with the independent observations from the Hawaii Ocean Time-series (HOT) (Dore et al., 2009), Bermuda Atlantic Time-series Study (BATS) (Bates, 2007) and The European Station for Time Series in the Ocean Canary Islands (ESTOC) (González-Dávila and Santana-Casiano, 2009) time series station.

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Table 1. The procedure of K-fold validation.

FFNN training | **FFNN testing**

1st iteration	**1992**	1993	1994	1995	**1996**	1997	1998	1999	…	**2012**	2013	2014	2015	**2016**	2017	2018	2019
2nd	1992	**1993**	1994	1995	1996	**1997**	1998	1999	…	2012	**2013**	2014	2015	2016	**2017**	2018	2019
3rd	1992	1993	**1994**	1995	1996	1997	**1998**	1999	…	2012	2013	**2014**	2015	2016	2017	**2018**	2019
4th iteration	1992	1993	1994	**1995**	1996	1997	1998	**1999**	…	2012	2013	2014	**2015**	2016	2017	2018	**2019**

Table 2. validation group

Validation group	Predictor
FFNN1	Indicators selected by stepwise FFNN algorithm
FFNN2	SST, SSS, $\log_{10}$(MLD), CHL-a, xCO_2, SST_{anom}, SSS_{anom}, $xCO_{2\ anom}$, CHL-a $_{anom}$, $\log_{10}(MLD)_{anom}$ (Landschuetzer et al., 2014)
FFNN3	SST, SSS, SSH, MLD, xCO_2, CHL-a, SSS_{anom}, SST_{anom}, SSH_{anom}, CHL-a $_{anom}$, MLD_{anom}, $xCO_{2\ anom}$, sLat, sLon, cLon (Denvil-Sommer et al., 2019)

3 Results and discussion

3.1 Biogeochemical provinces and corresponding predictors of pCO_2

11 biogeochemical provinces generated from the SOM method after the separated small 'island' was removed and the province separated by lands was divided manually (Fig. 3). The results of the stepwise FFNN algorithm in each province were shown in the Table 3. The indicators were listed in the order that the stepwise FFNN algorithm printed recommended predicators out. The indicator printed earlier was relatively more recommended and played an important role in the prediction of pCO_2 based on FFNN. Applying of these indicators as the predicators of surface ocean pCO_2 effectively decreased the predicating error between the FFNN outputs and pCO_2 values from validation samples, thus it is reasonable to consider that these indicators were highly related to the drivers of pCO_2 and its variability. Indicators representing sampling position were also listed as recommended predicators in some provinces, including latitude, longitude and sampling time, suggesting that relatively steady spatial or temporal variability pattern of surface ocean pCO_2 existed in these biogeochemical provinces. For example, month was considered as a recommended predicator in most provinces. Especially in the provinces covering the north Atlantic Ocean (P4 and P5), the parameter month was relatively more recommended. While pCO_2 in these areas regularly peaked and bottomed out in summer and winter (Takahashi et al., 2009;

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Landschutzer et al., 2016; Landschützer et al., 2020). Similarly, latitude and the sine and cosine of longitude were listed as recommended predicators of pCO_2 in most provinces, suggesting an obvious spatial distribution pattern of pCO_2, which was not learned sufficiently by the FFNN model from existing indicators and the indicators related to spatial position were applied as supplementary.

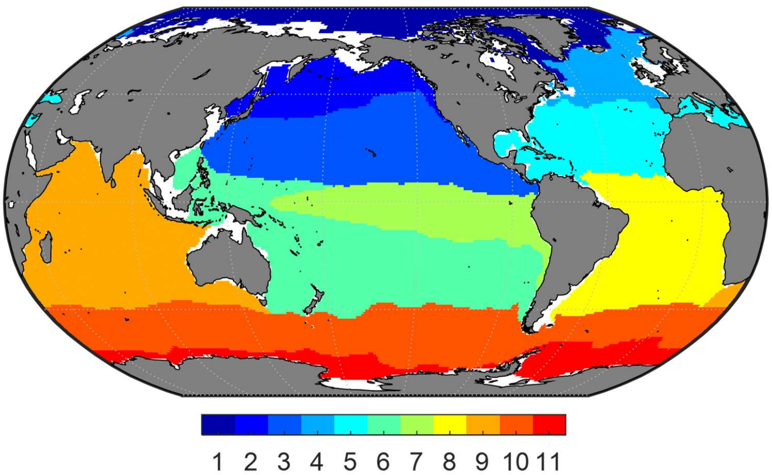

Figure 3. The map of biogeochemical provinces

As basic parameters highly related to the ocean environment, the temperature and salinity was considered as parts of the most important predictors of surface ocean pCO_2, and was applied in the pCO_2 prediction in almost all previous relating researches based on various method (Jo et al., 2012; Signorini et al., 2013; Landschuetzer et al., 2014; Marrec et al., 2015; Chen et al., 2016; Moussa et al., 2016; Chen et al., 2017; Laruelle et al., 2017; Zeng et al., 2017; Chen et al., 2019; Denvil-Sommer et al., 2019). The results of stepwise FFNN algorithm also supported this. Temperature was listed as a recommended predictor in all biogeochemical provinces, suggesting that temperature was the one of the most important drivers of pCO_2 and its variability in these provinces. Similarly, the result of stepwise FFNN algorithm proved the importance of salinity in the predication of pCO_2, which was also listed as a predicator in most provinces. In the province P1 located in the Arctic, the silicate concentration and temperature were considered as the most crucial predicator of pCO_2. The dry air mixing ratio of atmospheric CO_2 (xCO_2) and the monthly anomaly of xCO_2 were also recommended predicators in most of the biogeochemical provinces, suggesting that the exchange of CO_2 across the sea-air interface was also an important driver of surface ocean pCO_2. As a widely used predictor in the pCO_2 prediction, the chlorophyll-a concentration (CHL-

a) played an important role in fitting the influence of biological activities on pCO_2 in previous researches (Landschuetzer et al., 2014; Zeng et al., 2017; Laruelle et al., 2017; Denvil-Sommer et al., 2019). Especially in the Southern Ocean (province P10 and P11) the CHL-a was listed as the most recommended predicator in the result of stepwise FFNN algorithm. While in some other provinces (P1 and P5), the CHL-a were considered redundant that no effective decrease of MAE between FFNN outputs and pCO_2 measurements appeared when CHL-a data was used. Similar with the period that CHL-a was not available (represented by the subscript 'b'), the phosphate, nitrate, silicate or dissolved oxygen were recommended instead.

Table 3. Predicators in each biogeochemical province

Province	Predictors
P1	Silicate, SST, Wind speed, SSS, $\log_{10}$(MLD), SSS_{anom}, sLat, month, W_{vel}(65m), $\log_{10}(MLD)_{anom}$, xCO_2, cLon, Bathymetry, SSH
$P2_a$*	Nitrate, CHL-a, SSS, xCO_2, cLon, SST, $\log_{10}$(MLD), sLon, sLat, month
$P2_b$*	Nitrate, xCO_{2anom}, sLon, SST, sLat, $\log_{10}$(MLD), cLon, SSS, SSH_{anom}, DO, W_{vel}(195m), Bathymetry, Silicate
$P3_a$	$\log_{10}$(MLD), N_{mon}, SSH, SST, sLon, sLat, SSS, Bathymetry, month, $\log_{10}(MLD)_{anom}$, cLon, Surface pressure, W_{vel}(105m), CHL-a, DO, SSH_{anom}, $xCO_{2\,anom}$
$P3_b$	$\log_{10}$(MLD), xCO_2, sLat, sLon, SST, Surface pressure, cLon, SSS, W_{vel}(5m), N_{mon}, $\log_{10}(MLD)_{anom}$, month, Phosphate, $xCO_{2\,anom}$, W_{vel}(105m)
$P4_a$	month, sLat, cLon, SST, Year, CHL-a, DO, SSS_{anom}, W_{vel}(195m), SSH, $\log_{10}$(MLD), Bathymetry, SSS
$P4_b$*	month, xCO_2, DO, Wind speed, $\log_{10}$(MLD), W_{vel}(195m), sLon, Bathymetry, W_{vel}(5m), SST, Phosphate, Year, N_{mon}
P5	month, Year, SST, sLon, sLat, SSS, SST_{anom}, SSH, Bathymetry, W_{vel}(5m), cLon, W_{vel}(65m), $\log_{10}(MLD)_{anom}$
$P6_a$	SST, sLon, $xCO_{2\,anom}$, sLat, SSS, month, Phosphate, CHL-a, $CHL\text{-}a_{anom}$, W_{vel}(65m), $\log_{10}$(MLD), $\log_{10}(MLD)_{anom}$, Nitrate, Bathymetry
$P6_b$	xCO_2, sLat, SSS, SST, Phosphate, SLP, $xCO_{2\,anom}$, sLon, cLon, W_{vel}(105m), W_{vel}(65m), DO, Bathymetry, SSH, SAM
$P7_a$	Nitrate, xCO_2, sLat, SSS, SST, cLon, $xCO_{2\,anom}$, $\log_{10}$(MLD), sLon, CHL-a, Phosphate, W_{vel}(5m), W_{vel}(105m), W_{vel}(195m)
$P7_b$	SST, SSS, Year, sLat, month, cLon, SSH, Bathymetry, W_{vel}(65m), xCO_2
$P8_a$	sLat, $xCO_{2\,anom}$, SSS, $\log_{10}$(MLD), CHL-a, SSH_{anom}, W_{vel}(195m), cLon, SST, W_{vel}(65m), Bathymetry, Nitrate

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Province	Predictors
$P8_b$	SST, xCO_2, cLon, sLat, SSS, Silicate, SSH, log_{10}(MLD), sLon
$P9_a$	SST, cLon, sLat, Nitrate, W_{vel}(65m), log_{10}(MLD), SLP, CHL-a, Year, $log_{10}(MLD)_{anom}$, SSH_{anom}
$P9_b$	SLP, month, sLon, $xCO_{2\ anom}$, SST, Silicate, W_{vel}(65m)
$P10_a$	CHL-a, log_{10}(MLD), N_{mon}, SSS, SST, Bathymetry, SSH_{anom}, W_{vel}(5m), CHL-a_{anom}, xCO_2
$P10_b$	Wind speed, $xCO_{2\ anom}$, SSS, Phosphate, log_{10}(MLD), W_{vel}(65m), Bathymetry, SST, month
$P11_a$	CHL-a, sLon, Bathymetry, SSS, SSH, SST, Nitrate, cLon, sLat
$P11_b$	month, DO, SST, SSH, sLat, Nitrate, sLon, SSS, W_{vel}(195m), Silicate, SSHanom

*: Due to insufficient coverage of CHL-a data in the polar areas and during the period before 2002. The pCO$_2$ data in the province that CHL-a or CHL-a $_{anom}$ was selected as predicators was divided into two periods. The period that CHL-a data available was represented by the subscript 'a', such as $P2_a$, including global grids from 2002 to 2019 except polar grids in winter. The period that CHL-a data not available was represented by the subscript 'b', such as $P2_b$, including global grids from 1992 to 2001 and additionally some polar grids in winter from 1992 to 2019.

3.2 *p*CO₂ product

Based on the predicators given by the stepwise FFNN algorithm in each biogeochemical province, a FFNN size (representing the number of neurons in the hidden layer) improving validation was applied to further decrease the predication error. The MAE values based on same samples and FFNN model with different number of neurons were calculated, then the number of neurons corresponding to the lowest MAE were applied (Fig. 4a). The MAE in most provinces tend to decrease first and then increase when the number of neurons in the hidden layer of FFNN model increased from 10 to 70. Based on the variation of MAE with the number of neurons in the FFNN hidden layer, the optimal FFNN size in each province was considered as the number of neurons when the MAE was lowest. The result and corresponding MAE were shown in Fig. 4b. The MAE and RMSE of global estimates between predicted pCO$_2$ and measurements from SOCAT v2020 further decreased to 11.32 and 17.99 µatm respectively after applying optimal FFNN size in each province.

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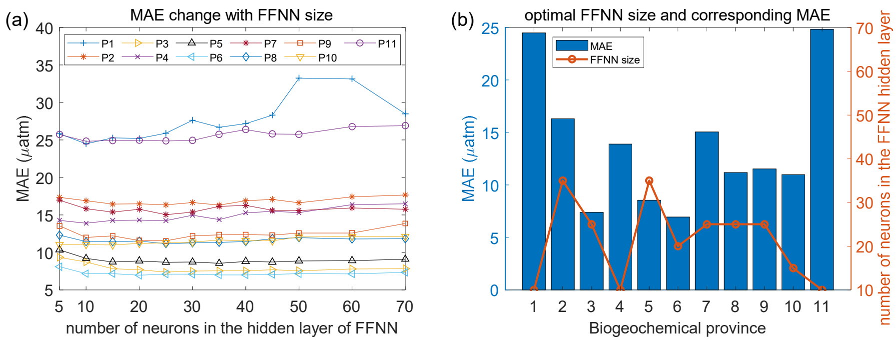

Figure 4. MAE of different FFNN size in each biogeochemical province.

Then the RMSE and mean residuals in each grid were calculated based the K-fold cross validation method. In most grids, the RMSE was lower than 10 μatm and the mean residuals was close to zero (Fig. 5). However, the prediction error in the north subpolar Pacific, the east equatorial Pacific and the Southern Ocean near the Antarctic continent was obviously higher than other areas. Distribution of mean residuals suggested that surface ocean pCO_2 in the Indian Ocean tend to be overestimated by the FFNN models. While in other regions the distribution of mean residuals was more discrete and no obvious pattern was found.

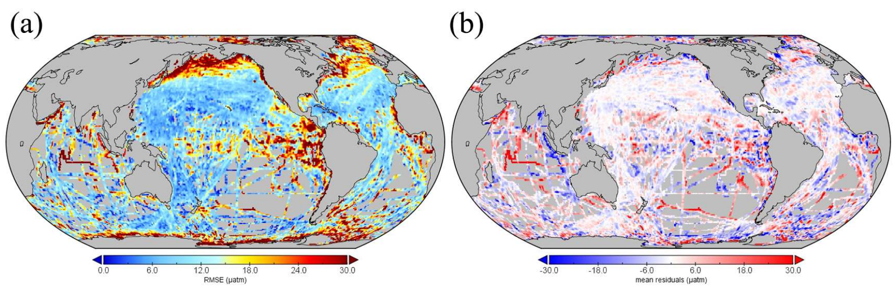

Figure 5. Global maps of (a) RMSE and (b) mean residuals between predicted pCO_2 and SOCAT observations

Based on stepwise FFNN algorithm and improved FFNN size in each province, a monthly 1°×1° grided surface ocean pCO_2 product from January 1992 to August 2019 was constructed. The interannual variability of global average pCO_2 was showed in the Fig. 6. The global open ocean average pCO_2 increased about 1.85 μatm per year from 1992 to 2019.

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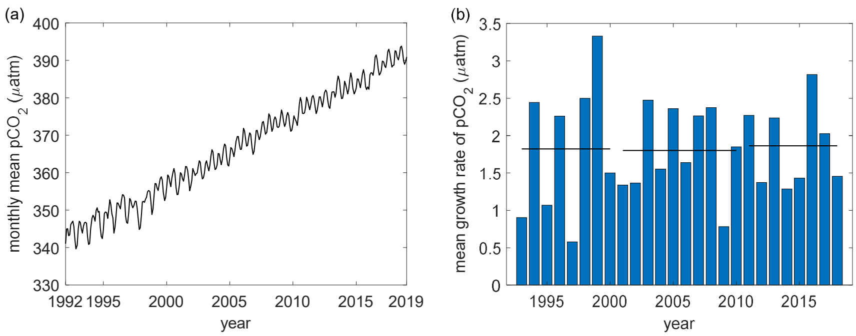

Figure 6. Interannual variability of global open-oceanic pCO_2 during 1992-2019. (a): global monthly mean pCO_2, (b): growth rate of global monthly mean pCO_2

3.3 Validation of the stepwise FFNN algorithm based on SOCAT samples

Validation based on the K-fold cross validation method suggested that most FFNN outputs were quite close to the pCO_2 values from SOCAT v2020 samples (Fig. 7). Comparing the results based on different combination of predicators, the results of FFNN1 (based on stepwise FFNN algorithm, this paper) and FFNN3 (based on 15 predicators from Denvil-Sommer, et al. 2019) were obviously more precise than that of FFNN2 (based on 10 predicators from Landschuetzer, et al. 2014). Where the plots in the result of FFNN1 was most concentrated along the y=x line, suggesting extremely close FFNN outputs with the measured pCO_2 values from SOCAT, with the RMSE of 17.99 μatm in the global open oceans. The RMSE of FFNN1 was lower than that of FFNN2 (22.95 μatm) and FFNN3 (19.17 μatm).

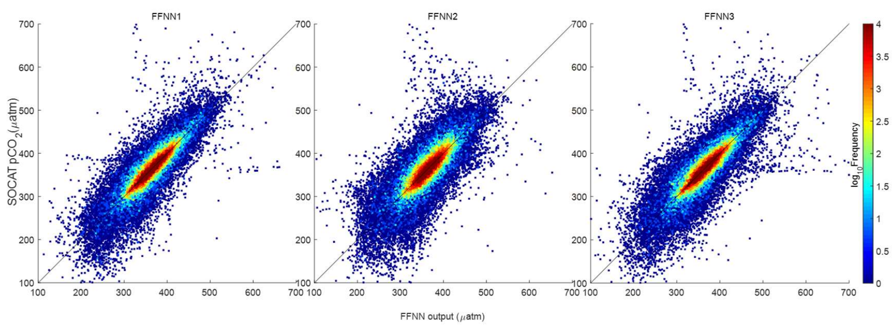

Figure 7. Comparing of FFNN predicted pCO_2 with SOCAT pCO_2. FFNN1 was based on predictors selected by the stepwise-FFNN algorithm. FFNN2 and FFNN3 were based on predictors from Landschuetzer et al., 2014 and Denvil-Sommer et al., 2019 respectively.

For specific comparison of accuracy in each province, the MAE of FFNN1 was lower in most provinces (Table. 4), except the relatively close results between the FFNN1 and FFNN3 in parts of provinces. Where the MAE of FFNN1 in the province

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P9 was significantly lower than that of the other validation groups, suggesting a better combination of predicators highly related to the drivers of surface ocean pCO_2 and its variability in the Indian Ocean. Compared with predicators of FFNN2 and FFNN3, the predicators of FFNN1 added surface pressure and W velocity of ocean currents, and abandoned the monthly anomalies of other indicators in the province P9. The low relevance between part of the monthly anomalies, such as SSS_{anom} and SSH_{anom}, may be responsible for significant lower MAE of FFNN1. Adding redundant indicators may cause misleading in the learning of FFNN model on the contrary. The MAE and RMSE difference between FFNN1 and FFNN3 in some provinces were relatively small, because predicators used in both FFNN1 and FFNN3 were related to main drivers of pCO_2, such as CHL-a, xCO_2 and MLD.

Table 4. Performance of the pCO_2 prediction based on different predicators

Province	FFNN size	MAE (μatm)			RMSE (μatm)		
		FFNN1	FFNN2	FFNN3	FFNN1	FFNN2	FFNN3
P1 (9856)	10	24.50	32.32	26.87	32.27	43.68	35.08
P2 (30516)	35	16.32	20.63	16.67	24.32	29.87	25.03
P3 (56367)	25	7.39	12.16	7.95	11.33	17.75	11.88
P4 (29595)	10	13.89	16.91	14.73	21.06	24.29	22.27
P5 (45358)	35	8.55	12.28	9.00	12.80	17.86	13.72
P6 (31803)	20	6.96	9.94	7.24	9.86	14.64	11.00
P7 (11233)	25	15.05	19.55	15.49	20.98	27.61	21.10
P8 (10259)	25	11.19	15.07	12.43	17.10	20.87	17.66
P9 (7440)	25	11.54	13.78	15.49	17.15	22.89	28.29
P10 (21206)	15	11.00	11.76	12.14	16.61	17.22	17.66
P11 (10683)	10	24.84	29.26	25.74	34.73	40.42	35.22
Global (264316)		11.32	15.08	12.06	17.99	22.95	19.17

(FFNN1 was based on predictors selected by the stepwise-FFNN algorithm. FFNN2 and FFNN3 were based on predictors from Landschuetzer et al., 2014 and Denvil-Sommer et al., 2019 respectively.)

3.4 Validation based on independent observations

The FFNN outputs based on different combination of predicators were compared with independent observations from the Ocean Time-series (HOT) (Dore et al., 2009),

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Bermuda Atlantic Time-series Study (BATS) (Bates, 2007) and The European Station for Time Series in the Ocean Canary Islands (ESTOC) (González-Dávila and Santana-Casiano, 2009) (Fig. 8). The interannual variability and seasonal pattern of pCO_2 in the grids the HOT station located from different validation groups were similar and close to the observations from the HOT, which was located in the province P3. From 1992 to 2019, the RMSE between FFNN1 outputs and HOT observations was only 9.29 µatm, lower than the 10.85 µatm of FFNN2 and the 10.70 µatm of FFNN3.The monthly mean pCO_2 of FFNN2 during winter was obviously lower than the HOT observations and pCO_2 values of other validation groups, while the FFNN1 and FFNN3 outputs were closer to the HOT observations. MAE between predicted pCO_2 and HOT observations were also lower in the validation group FFNN1, which was only 7.17 µatm, compared to the 8.61 µatm of FFNN2 and the 8.44 µatm of FFNN3. Higher bias generated in the winter bottom and summer peak, which was showed more obviously in the monthly average of pCO_2 (Fig. 8b). Compared with other validation groups, the result of FFNN1 was closer to the monthly average values of the HOT observations. Same conclusion can be obtained in the ESTOC and BATS station located in the province P5. The RMSE between FFNN1 outputs and independent observations were 13.03 µatm in the BATS station and 11.35 µatm in the ESTOC station, lower than that of other validation groups. The RMSE between FFNN2 outputs and independent observations was 16.15 µatm in the BATS station and 14.51 µatm in the ESTOC station. For the group FFNN3, the RMSE was 13.09 µatm in the BATS station and 13.01 µatm in the ESTOC station. All results were extremely close to the independent observations, but the RMSE and MAE of FFNN1 were lower. Similar with the situation in the HOT station, the FFNN1 was most close and the FFNN3 second. Based on the better performance of FFNN1, in which the predicators selected by stepwise FFNN algorithm were used, we may conclude that the stepwise FFNN algorithm can effectively find better combination of predictors to fit the diver of surface ocean pCO_2 and obtained lower error.

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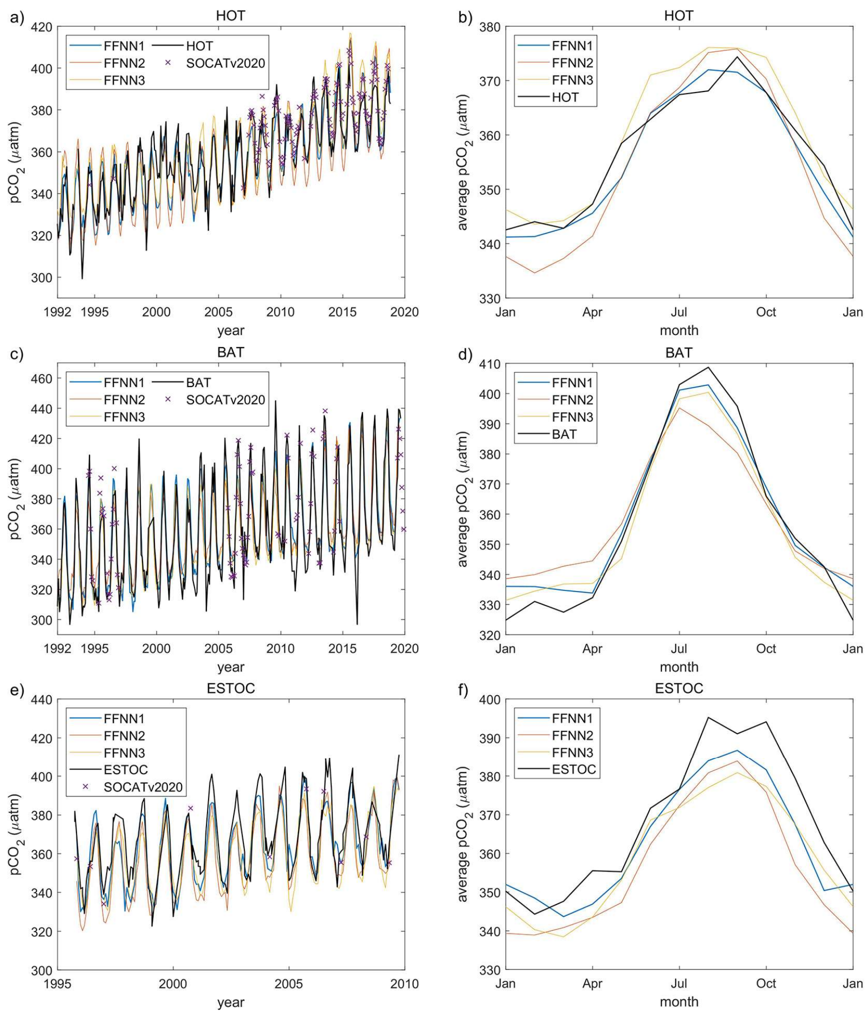

Figure 8. Validation based on independent observation from time series stations. a) and b): the Hawaii Ocean Time-series (HOT) (Dore et al., 2009); c) and d): the Bermuda Atlantic Time-series Study (BATS) (Bates, 2007); e) and f): the European Station for Time Series in the Ocean Canary Islands (ESTOC) (González-Dávila and Santana-Casiano, 2009) time series station. FFNN1 was based on predictors selected by the stepwise-FFNN algorithm. FFNN2 and FFNN3 were based on predictors from Landschuetzer et al., 2014 and Denvil-Sommer et al., 2019 respectively. SOCATv2020 represents the monthly mean pCO_2 of SOCAT observations in the corresponding grids of each time series station.

3.5 Climatological spatial distribution

The climatological average distribution of pCO_2 suggested a significant spatial variability (Fig. 9), which is consistent with the average distribution of SOCAT observations. In the Pacific Ocean, the high pCO_2 areas showed by the stepwise-FFNN product (Fig. 9b), including the equatorial areas, east temperate areas and north subpolar areas, were highly consistent with the SOCAT datasets (Fig. 9a). Similarly, the distribution of pCO_2 in the Atlantic Ocean and the Indian Ocean was also close. However, the stepwise-FFNN product suggested lower pCO_2 average values in the Arctic and higher values in the Southern Ocean near the Antarctic continent. Compared with previous climatology product (Landschützer et al., 2020), the global distribution pattern of surface ocean pCO_2 was basically well consistent. Inconsistent spatial distribution also existed in the Arctic and parts of the Southern Ocean near the Antarctic continent. The differences between stepwise-FFNN product and previous climatology product may be caused by differences in methods or SOCAT dataset versions used. While lower average values of the SOCAT dataset in the Southern Ocean may be caused by the undersampling in winter. The global spatial distribution pattern of the stepwise FFNN pCO_2 product was basically well consistent with previous climatology product and SOCAT dataset, suggesting that pCO_2 predicting based on regional different predictors selected by the stepwise FFNN algorithm was credible.

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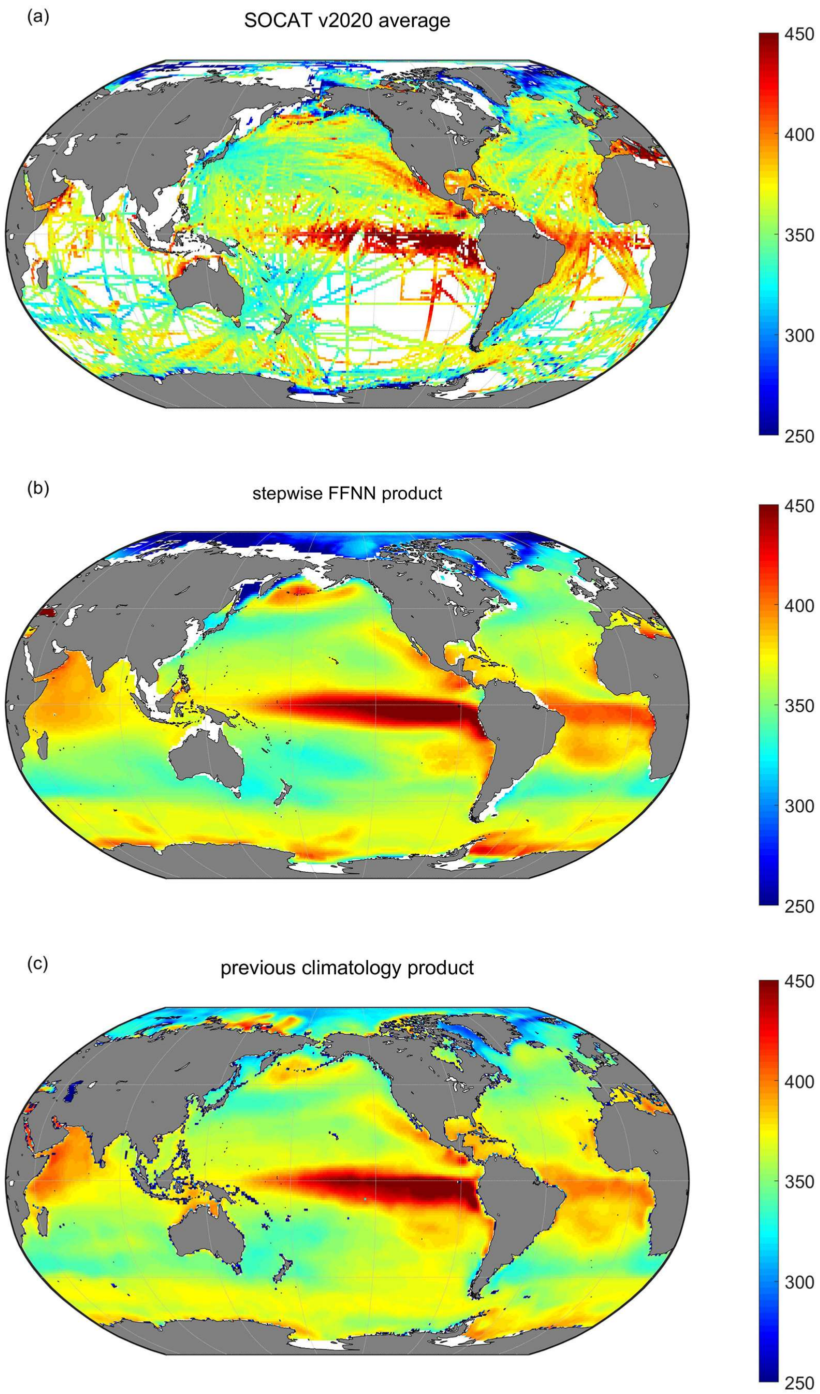

Figure 9. Comparison between long term average of a): SOCAT v2020 dataset, b): the stepwise FFNN pCO_2 product and c): previous climatology product adapted from Landschützer et al., 2020.

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4. Conclusions

A stepwise FFNN algorithm was constructed to decreasing the predicating error in the surface ocean pCO_2 mapping by finding better combinations of pCO_2 predicators in each biogeochemical province defined by SOM method. Comparing with the performance of FFNN based on predicators same with previous researches, the RMSE decreased when using predicators selected by the stepwise FFNN algorithm in all provinces, suggesting that the stepwise FFNN algorithm was capable to find better combination of predicators. In addition, validation based on independent observations from HOT, BATS and ESTOC time series stations also proved the better performance of FFNN based on predicators selected by the stepwise FFNN algorithm. We further decreased the MAE and RMSE of global estimates to 11.32 and 17.99 μatm by improving the number of neurons in the hidden layer of FFNN. Then a monthly 1°×1° gridded global open-oceanic surface ocean pCO_2 product from January 1992 to August 2019 was constructed, based improved FFNN size and the predicators selected by stepwise FFNN algorithm. In this study, regional specific combination of predicators was first applied in the global surface ocean pCO_2 mapping. The result of the stepwise FFNN algorithm was also capable for analyzes of driving based on the ranking of relative importance of each predicator. The more important predicator, which played a more important role in decreasing the predicting error, will be selected earlier and listed at the front of the recommended predicator list. In the future work, the stepwise FFNN algorithm will be attempted in the mapping of other parameters, such as total alkalinity and pH, to provide more sufficient data support for studies on ocean acidification and carbon cycling.

Code and data availability

The stepwise FFNN algorithm (as a .m file for MATLAB) and the global 1°×1° gridded surface ocean pCO_2 product since from January 1992 to August 2019 (as a NetCDF file) generated during this study is available from the Institute of Oceanology of the Chinese Academy of Sciences Marine Science Data Center at http://dx.doi.org/10.12157/iocas.2021.0022.

Author contribution

Ma Jun, Yuan Huamao and Duan Liqin collected the dataset of pCO_2 predicators, and Qu baoxiao and Wang Yanjun was contributed in the synthesis of datasets. Zhong Guorong, Li Xuegang and Song Jinming designed the predicator selection algorithm and performed the reconstruction of pCO_2 product. Wang Fan, Zhang Bin, Sun Xiaoxia, Zhang Wuchang, and Wang Zhenyan were contributed in the further improving. Zhong

Guorong prepared the manuscript with contributions from all co-authors.

Competing interests

The authors declare that they have no conflict of interest.

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