

Reviewer 1

The authors developed a new ML approach to reconstruct global surface ocean pCO₂ that considers an impact of different predictors in different ocean regions. Based on Self-Organizing Map method authors defined 11 biogeochemical provinces. A stepwise FFNN regression algorithm was applied to each of these provinces to establish a set of predictors that are highly responsible for pCO₂ variability in considered province. Based on selected predictors and analysis of FFNN size (number of neurons) a monthly 1°x1° surface ocean pCO₂ product from 1992 to 2019 was constructed. The results show a good agreement with validation data and independent observations.

I found this work well-organized and easy to read. It was interesting to see new predictors (phosphate, nitrate, silicate, dissolved oxygen) and their role in pCO₂ variability. The authors presented important results for the Indian Ocean where due to the lack of observations different methods show their disagreements.

Response: Thank you very much for your appreciation and very valuable suggestions to improve the manuscript!

Below, I listed several points that need to be clarified before publication.
Comments:

- **Boundaries between provinces.** In the text we can find “To obtain a smoother distribution, we defined that the grid within 5 1x1 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.” Please could you clarify what you mean by “only counted once in the validation”? Is only an output from one province used in the validation? If yes, how do you chose a province from which you take an output?

Response: Thank you for pointing out this unclear description. This definition was only applied to increase training samples near the province boundary. However, the range of validation and interpolation in each province will not change. Figure S1 was added in the supplement to make this definition easier to understand. And the text in manuscript was modified as:

“To obtain a smoother distribution, we defined that the area within 5 1x1 grids of province boundaries as a ‘boundary area’. Samples in the boundary area will be used as training samples in all adjacent provinces (Fig. S1). But this definition does not change the actual spatial coverage of each province, only brings more training samples near the province boundary.”

- **Independent observations. Please could you provide geographical positions and period of stations used as independent observations?**

Response: The HOT station is located in 22° 45'N, 158° 00'W and observations started since October 1988. The BATS station is located in 31°50'N, 64°10'W and observations are from October 1988 to December 2019. The ESTOC station is located in 29°10'N, 15°30'W and observations from 1995 to 2009 were used. The information above was added in the validation section.

- **Set of selected predictors. In table 3 authors presented two sets for most of the regions that depends on the availability CHL-a data. Please could you present more explicitly that the final product is built on two FFNNs, one trained for the period 1992-2001 based on one predictors set and another – for 2002-2019 based on the second predictors set?**

Response: Thanks for your suggestion. A description was added in the section 2.4 pCO₂ product as “Then the final product was built based on two FFNNs, one trained for the period 2002-2019 using one predictor set including CHL-a or CHL-a anom, and the second one for the 1992-2001 using the second predictor set without CHL-a and CHL-a anom.”

- **More explicit figures' captions. Please provide more explicit figures' captions, period of presented results, or results averaged over xxxx-xxxx, what are horizontal lines in Fig.6b?**

Response: Thanks for your suggestion. The horizontal line was the average pCO₂ growth rate over each decade (1992-2000, 2001-2010 and 2011-2019). This figure was moved to supplement now.

- **Not correct conclusion. On page 15 lines 375-379 authors concluded that the difference between FNN1 and FFNN3 is relatively small, because predictors used in FFNN1 and FFNN3 were related to main drivers of pCO₂, such as CHL-a, xCO₂ and MLD. However, same drivers are used in FFNN2. Thus, it cannot explain why FFNN2 shows higher differences with observations.**

Response: Thank you for pointing out this mistake. After reconsidering this issue, I think the application of latitude and longitude as predictors of pCO₂ may be the reason why FFNN2 shows higher MAE and other validation groups shows relatively closer results. For example, in the province P10 that latitude and longitude were considered not good predictors by the stepwise FFNN algorithm, the three validation groups show significant closer results than that

in other provinces. While in other provinces, latitude and longitude were used as predictors in the FFNN1 and FFNN3, decreasing the MAE and RMSE. The text was corrected as “The MAE and RMSE difference between FFNN1 and FFNN3 in some provinces were relatively small. The reason for higher MAE and RMSE showed by the FFNN2 may be the application of latitudes and longitudes as predictors in both the FFNN1 and FFNN3 but not in the FFNN2. In the province P10, latitudes and longitudes were considered not good predictors by the stepwise FFNN algorithm and the results of three validation groups were extremely close.”.

- On page 18 line 430 authors said that the pattern of reconstructed pCO₂ climatology was close to SOCAT in the Indian Ocean. I would say that it is not so close to mention it in this sentence.

Response: Thanks for your suggestion. The inaccurate description was now removed.

- Page 10 lines 298-300: For better structure of paragraph the sentence “In the province P1 located in the Arctic, the silicate concentration and temperature were considered as the most crucial predictor of pCO₂.” could be moved at the end of paragraph where authors mentioned the phosphate, nitrate, silicate, etc.

Response: Thanks for your suggestion. The sentence was now moved at the end.

- Page 13 lines 336-337: The sentence about results in the Indian Ocean can be removed if you put the Indian Ocean in the previous sentence, or please add “Also” at the beginning of the sentence dedicated to results in the Indian Ocean.

Response: At the beginning of the sentence “Also” has been added now.

- Page 16 lines 390-392: Please could you reformulate this sentence (“The interannual variability and seasonal pattern..”) as it is difficult to read?

Response: The sentence was modified as “Compared with the independent observations from the HOT station, the three validation groups both show close results, which were also similar with each other in the seasonal and interannual variability of pCO₂”.

- Page 18 lines 432-436: two sentence can be combined: “Compared with previous climatology product (Landschuster et al., 2020), the

global distribution pattern of surface ocean pCO₂ was basically well consistent: inconsistent spatial distribution also existed in the Arctic and parts of the Southern Ocean near the Antarctic continent.”

Response: Thanks for your suggestion. The two sentences now have been combined.

Typo:

Page 2 line 41: “surface ocean pCO₂” should be replaced by “Surface ocean pCO₂”.

Page 9 line 261: “validation group” should be replaced by “Validation group”.

Page 13 line 332: “Based the K-fold” should be replaced by “based on the K-fold”.

Page 20 line 459: “based improved FFNN size” should be replaced by “based on improved FFNN size”.

Response: Thank you for pointing out these mistakes. These mistakes have been corrected now.

Review 2

General comments:

The stepwise FFNN looks like a innovative new approach to enhance the widely popular SOM-FFNN method. The stepwise method is tested using a very comprehensive list of predictors used elsewhere in the literature. The method building component looks thorough, congrats. The prediction of pCO₂ based on region-specific predictors selected by the stepwise FFNN algorithm will be a valuable tool when moving to higher resolution, inside regional studies, or getting closer to shore. There are a number of grammatical errors that will need to be cleaned up by the authors or the journal team.

Response: Thank you very much for your appreciation and very valuable suggestions to improve the manuscript!

Specific comments:

1 Introduction

Line 66-82: Appreciate the list of previous works and predictor data used by each, provides justification for use in the stepwise FFNN. Would like to see one more sentence relating use of different predictors leading to varying marine sink estimates.

Response: Thanks for your suggestion. In previous researches, not only different predictors, but also different methods were used. Thus, the differences in estimate of marine carbon sink between previous researches were not only caused by use of different predictors. In addition, there is almost no such research that focusing on the influence of predictor differences on marine sink estimate.

2 Methodology

2.1 Data

Line 106-122: Are all these products retrieved at the same resolution? Are they upscaled or downscaled at all to your needs?

Response: Most of these products were retrieved at 1° × 1° resolution. Some products retrieved at higher resolution were downscaled to 1° × 1° resolution. This description has been added at the end of the 2.1 Data section and supplement.

Line 122: “In addition, 8 parameters....” Thanks for listing after this sentence. Which previous research used these as predictors in observation-based pCO₂ estimates? List and provide citations like in the introduction. Or is the inclusion of these predictors’ novel? If so, highlight

that.

Response: These parameters have not been used as predictors in observation-based pCO₂ estimates in previous researches yet, but nutrients and dissolved oxygen have been used as predictors in observation-based estimates of total alkalinity and DIC. The citation has been added.

2.2 Biogeochemical provinces defined by the Self-Organizing Map

Line 134: These SOM predictors exclude most of the FFNN predictors discussed in the introduction. Was there a reason why “biological” predictors (i.e., nutrients and oxygen) are weighted so heavily in the SOM selection? Were more physical predictors (i.e., mixed layer depth, etc.) used in SOM testing to optimize provinces? Or similar to previous work (Landschützer), using published pCO₂ climatology as a predictor to determine provinces?

Response: Thanks for noting this problem. Actually, we also used mixed layer depth, sea surface height and pCO₂ climatology from Landschützer, 2020, but mistakenly lost in the text. The description about predictors has been corrected now.

Line 135: Just out of curiosity, did the configuration (3-by-4 size) make much of a difference to SOM province distribution?

Response: In the early work, 4-by-4 or 4-by-5 size were also attempted. Increasing size led to appearance of small provinces inside main provinces, but the distributions of main provinces were similar. To simplify the SOM boundary issues, we choose the 3-by-4 size with less provinces.

Line 141: The 200 m depth boundary is fairly close to shore. Is this a commonly used open oceanic / coastal ocean boundary? If so citations from other studies here.

Response: It is not a commonly used boundary. In previous researches focusing on coastal pCO₂ reconstruction, the boundary was defined as 1000m depth or 300 km offshore. We defined the boundary as 200m depth because the SOCAT samples with high predicting error were mainly located in areas shallower than 200m.

Line 144: Unique way to address the SOM boundary issue. Cool.

Response: Thank you for your appreciation.

2.3 Stepwise FFNN algorithm

Line 152-163: Clarify. Was the mean absolute error used for the internal MATLAB neural network performance loss function (in the training targets and validation targets steps used to end training), also / or as a means for evaluating the FFNN output pCO₂ product to withheld data?

Response: The MAE was used for performance loss function, and also in the validation of pCO₂ product using a K-fold cross validation method.

Line 172: "...referred to as indicators pool (Start in Fig. 1),..." Keep coming back to this Figure throughout if you can. Makes it easier to read and connect to the Figure.

Response: Thank you for your suggestion. More annotations have been added in the description.

Figure 1: More sub boxes (dotted lines), connected to text could also make it easier to follow. Steps between loop 1 and loop 2, steps between loop2 and end.

Response: Thank you for your suggestion. More sub boxes have been added in the Figure 1.

2.4 pCO₂ product

Line 227: Reason why 10 and 70 are chosen? Is there a possibility that even in smaller provinces 10 neurons could lead to overfitting? The polar regions are set right at 10.

Response: We test the number of neurons from 5 to 300. The MAE continuously increasing after 70. The variation of MAE would be difficult to see clearly if all spots were showed, so the results after 70 were omitted. Seems the way the result shows may be misleading, so we redrew the Fig.4a. Not just focusing on overfitting, too few neurons may lead to insufficient learning capacity for complex nonlinear relationship, so we tested the performance of FFNN with different number of neurons.

Line 231: Does this vary neuron number test really limit overfitting? Taking the lowest MAE from the internal train/validation split during FFNN training step just means it is likely replicating training data well and due to random split inside autocorrelated validation data this doesn't change much. Being clear in Line 152-163 about how / when MAE is used to evaluate could clear this up.

Response: The MAE used here was calculated using a K-fold cross validation method grouping by year. The training data and validation data were taken from

different years and were relatively independent. The MAE theoretically tend to increase when insufficient learning capacity due to too few neurons or overfitting problem due to too many neurons appear. The result shows that the MAE did increase when the number of neurons was lower than 10 and higher than 100.

2.5 Validation

Line 237: Unique use of the K-fold cross validation method grouping by year.

Response: Since samples within 500 km in the same period were correlated, grouping by year makes the training data and validation data relatively more independent.

3 Results and discussion

3.1 Biogeochemical provinces and corresponding predictors of pCO₂

Table 3: Add more to the caption on the order of the predictors listed.

Response: Thank you for your suggestion. The caption has been modified.

3.2 pCO₂ product

Line 317: Does this mean you first went through the stepwise FFNN process using the same neuron number? Then when the best predictors where determined you used the varying neuron number test (from 10-70) to find the best neuron number? Then you used the K cross validation to test robustness? Clarify. Link to back to Figure 1 if you need to.

Response: Yes, the stepwise FFNN process use the same neuron number. Since the result of varying neuron number test shows there is almost no insufficient learning capacity or overfitting problem when the number of neurons was in 10-70 and the MAE differs a little. Any number of neurons in this range was considered suitable. Although a loop of “stepwise FFNN – neuron number test – stepwise FFNN -” to use different number of neurons in the stepwise FFNN process may further decrease the predicting error, the effect was not so significant and a stable end is not easy to find. In the future work the role of the varying neuron number test may be reconsidered, but now it is used for avoiding insufficient learning capacity or overfitting problem in spite of the low possibility of appearance, and decreasing the predicting error slightly.

Figure 4: Still not sure on this test limiting overfitting. Looks like they all (except at the poles maybe because it is not well constrained...? As in your Table 4) just level out. Using the same FFNN predictors and the same targets how reproducible is this Figure? Or is it dependant on the initialization on that run?

Response: The Fig. 4a has been modified to show the additional result of 70-300. The MAE increased after 100. In MATLAB we used "setdemorandstream(pi)" to set initial state stable, thus the result using the same FFNN predictors and the same targets is completely reproducible.

Line 334: Good to state this up front. Other than these regions it does look good. However, if the goal from the introduction is get at the air-sea flux, how important are these regions for the global marine CO₂ flux? Suggest in conclusions what could be done in the future to improve these regions?

Response: The east equatorial Pacific is the most important CO₂ source, while the subpolar Pacific was a sink in summer and a source in winter. The CO₂ flux in the Southern Ocean near the Antarctic continent was near zero due to ice cover. For the future work to improve these regions, maybe more parameters related to biological activities, El Niño and La Niña, or remote sensing parameters will be added to constrain the pCO₂ in these regions.

Figure 6a: Would be nice to also have the atmospheric xCO₂ product on this Figure for comparison.

Response: Thank you for your suggestion, the atmospheric CO₂ has been added.

3.4 Validation based on independent observations

Line 395: Nothing is obvious to every reader. Remove and clarify.

Response: Thank you for your suggestion. The unbefitting description has been removed.

Line 442: "... was credible." Is consistent with and improves upon? Readers should want to believe in what you did! Got to sell it a bit!

Response: Thank you for your suggestion. The text has been modified as "suggesting that pCO₂ predicting based on regional different predictors selected by the stepwise FFNN algorithm was better than that based on the globally same predictors."

4. Conclusions

Line 447-465: This needs a bit of a rework. Feels like recycled sentences from throughout. What should readers take away from your work? How can this approach be applied in other studies? Who benefits from this improvement? Where is more work needed (e.g., polar regions), how could improvements be made?

Response: Thank you for the suggestion. This part has been rewritten as “A stepwise FFNN algorithm was constructed to decreasing the predication error in the surface ocean pCO₂ mapping by finding better combinations of pCO₂ predictors in each biogeochemical province defined by SOM method, based on which a monthly 1°×1° gridded global open-oceanic surface ocean pCO₂ product from January 1992 to August 2019 was constructed. Our work provided a statistical way of predictor selection for all researches based on relationship fitting by machine learning methods, and shows that using regional-specific predictors selected by the stepwise FFNN algorithm retrieved lower predicting error than using globally same predictors. This stepwise FFNN algorithm can be also used in pCO₂ mapping researches for higher resolution and coastal regions, and also in other data mapping researches using SOM or other region dividing method. The prepare work was only collecting as many parameters, which are possibly related to the target data and need to be sufficiently available in time and space. However, high predicting error in special regions still remains to be improved, such as polar regions and equatorial Pacific. Since the result of the stepwise FFNN largely depends on the way biogeochemical provinces divided, improving of SOM step is still necessary. Besides, the FFNN can be replaced by any suitable type of neural networks. A possible way to improve the performance of stepwise FFNN algorithm is to modify the structure of FFNN or to use better networks.”.

Reviewer 3

This manuscript uses a stepwise feed-forward neural network (FFNN) to identify an optimal feature for the prediction of ocean pCO₂. The authors first use a self-organizing map (SOM) to cluster the ocean into 12 provinces base on a suite of climatological features. An optimal parameter set from a set of 33 predictors is determined for each province. The authors use this knowledge to create a monthly product of ocean pCO₂ from 1992-2019 at a 1x1 spatial resolution. Identifying optimal parameters is useful, especially for high-resolution regional products. Using a NN-based stepwise regression technique to identify the parameters is novel and something I have not seen before. I think this manuscript is a useful contribution to the field. However, the manuscript needs some improvements. The manuscript is well organized, but moving some text to tables and rearranging some paragraphs will make the manuscript easier to follow. The figures are appropriate but the figure legends need more clarifying text.

Response: Thank you very much for your appreciation and very valuable suggestions to improve the manuscript!

Below are specific line comments.

L38: What are the differences and how were the estimates made?

Response: The average global ocean sea-air CO₂ flux estimated by sea-air pCO₂ differences using different pCO₂ products differ from -1.55 to -1.74 PgC yr⁻¹ during 2001-2015, and the differences in individual years reached nearly 0.6 PgC yr⁻¹ (Rödenbeck et al., 2014; Iida et al., 2015; Landschützer et al., 2014; Denvil-Sommer et al., 2019). These estimates were made by multiplying sea-air pCO₂ differences by piston velocity, seawater density and CO₂ solubility, based on pCO₂ products constructed using statistical interpolation or machine learning methods. More specific description was added in the manuscript.

L41: I would consider rephrasing the “Surface ocean pCO₂ is ...” sentence to something like “The magnitude and direction of the flux is largely set by the air-sea pCO₂ difference.” I think this is a nice lead-in to the next sentence. I would avoid saying “in the data-based method” because this is something that is true in the real world too.

Response: The sentence has been rephrased according to the suggestion.

L64-66: Consider expanding on this idea and explaining why each feature was chosen. Each feature can be considered a proxy for a process

influencing pCO₂:

SST and SSS --> solubility

Chl-a --> phytoplankton uptake

MLD --> entrainment

xCO₂ --> Henry's law

I think a description of this will be useful for some readers

Response: Thank you for the suggestion. Additional description about the selection of each feature has been added.

L66-78 : A table could make this list of features easier to read. I suggest a table of the features, references that use each feature, and maybe the physical process that each feature is a proxy for.

Response: A table has been added in the supplementary, listing all features used and describing the references using the feature, data products used, spatial and temporal coverage.

L100: I think “conversion” is more appropriate than “transition” here.

Response: Thank you for the suggestion. The word “transition” was replaced.

L102: I like that you included units for the gas constant, please include units for each term (pCO₂, fCO₂, P, etc.)

Response: The units were added in the description. The sentences were modified as “where fCO₂ and pCO₂ are in micro-atmospheres (μatm), P is the total atmospheric surface pressure (Pa) using the National Centers for Environmental Prediction (NCEP) monthly mean sea level pressure product (Dee et al., 2011), and T is the absolute temperature (K). R is the gas constant (8.314 J K⁻¹ mol⁻¹). Parameters B (m³ mol⁻¹) and δ (m³ mol⁻¹) are both viral coefficients (Weiss, 1974).”

L106: I am unsure what “parts of indicators” means. I think this can be removed and replaced with something like “Predictors used in this study were chosen from previously published ocean pCO₂ products.”

Response: This selection was supposed to show most predictors used in this work were chosen from previously published ocean pCO₂ products, and some predictors were first used in the pCO₂ reconstructing. The sentence has been modified as “In this work, total 33 indicators were used. Where 25 indicators were chosen from previous researches of surface ocean pCO₂ reconstruction ...”

L109: Should this be Cheng et al. (2017)?
<https://www.science.org/doi/10.1126/sciadv.1601545>

Response: The citation of temperature data is Cheng et al. (2016) and Cheng et al. (2017), and the citation of salinity data is Cheng et al. (2020). The citation has been corrected.

L109-122: consider putting these features into a table for ease of reading.

Response: Thank you for the suggestion. A table has been added in the supplement, listing all features used and describing the references using the feature, data products used, spatial and temporal coverage.

L119: This is just a note that ERA interim has been deprecated in favor of ERA5.

Response: Because the temporal coverage of pCO₂ product in current version was only in 1992-2019. The ERA5 product will be used instead of ERA interim in the future version when other data product is sufficiently available for the reconstruction of pCO₂ after 2019.

L135: Why were 12 provinces chosen?

Response: In the early work, different number of provinces such as 16 or 20 were also attempted. Increasing number led to appearance of small provinces inside main provinces, but the distributions of main provinces were similar, such as provinces covering north Pacific, north Atlantic, equatorial and polar areas. In addition, more provinces lead to less SOCAT samples in each one province. So, we used as few as possible provinces to make sure that there are sufficient training samples in each one province.

L138: Please be specific here. How were island provinces defined? Having less than X pixels? For completeness, please indicate where this island province was and what it was merged with. How were island provinces quantified? Having less than X pixels? Maybe a better phrasing is something like: “SOM-based provinces needed to meet the following criteria: 1. contain more than X pixels. 2. co-locate with at least X SOCAT observations. Provinces that do not meet the criteria were merged with the dominant neighboring province.

Response: Thank you for the suggestion. Provinces with connected pixels less than 10 and provinces with SOCAT observation less than 1000 were define as island provinces, and then merged with nearest provinces. The more specific description has been added.

L139: “provinces covering area separated by land.” please explain this or give an example.

Response: The province P3 covering north temperate Pacific and the province P5 covering north temperate Atlantic were set as one province in the original output of SOM, but were mainly separated by The North American continent. So, we divided the province into two new provinces. Same process was carried out in the northwest Pacific, Mediterranean and so on. The more specific description has been added.

L141: Is 200m a typical definition for the coast? Can you please point to other studies that use this definition or indicate why this was chosen.

Response: It is not a widely used definition and different definition were used in previous researches. For example, 1000m depth and 30 salinity as boundary was used in Zeng et al., 2014, and 500m depth as boundary was used in Telszewski et al., 2009. Researches focusing on coastal pCO2 used a boundary of 1000m depth/300km offshore (Laruelle et al., 2017). We used 200m depth as boundary because the grids with high predicting error were mainly located in areas <200m depth.

L144: Have you tried different predictions to test this idea?

Response: We have compared the result using different predictors with the result using same predictors in all provinces. more obvious border lines appeared in some regions when using different predictors in each province, but we are not sure whether it is caused by application of a certain predictor or by the differences of predictors between neighboring provinces.

L145: Please clarify this sentence. I am unsure what this means.

Response: The text was rephrased and more description was added in the supplement. To obtain a smoother distribution, we defined that the area within 5 1x1 grids of province boundaries as a ‘boundary area’. Samples in the boundary area will be used as training samples in all adjacent provinces. This definition brings more training samples near the province boundary for each province, while these samples originally belong to other provinces. However, in the validation process of each province, the validation samples of each province were not change by the definition of boundary area. Also, the interpolation area of each province was not changed.

L151: Consider replacing this with a definition of what the stepwise part means. I am not too familiar with stepwise regression and a couple of

sentences describing what the stepwise part means could be beneficial to readers. Since this approach is integral to the paper it is important that it is defined well.

Response: Thank you for the suggestion. The sentence was replaced by “In the stepwise part, predictors of pCO₂ are going to be added and removed one by one, and which predictors will be finally used in the pCO₂ predicting is determined according to the real-time change of predication error.”

L200: This paragraph may be more appropriate at the beginning of this section

Response: Thank you for the suggestion. The paragraph has been moved to the beginning.

L210: does the result change significantly for depending on your choice of random number?

Response: The way that initial bias and weights matrixes of a FFNN randomly assigned depends on the random number stream. The result basically changed slightly when the initial state or the way testing sample group divided changed. For example, if 10 predictors were selected in the stepwise part, the last 2-3 predictors may change when the initial state of FFNN changed.

L225: could cite figure 4a. I am curious if you tried deeper networks with more than 1 layer?

Response: We test FFNN with two hidden layers. The result when using two hidden layers and 25 neurons in each layer was similar with the result using 125 or more neurons in one hidden layer. But we did not test more neurons in two hidden layer or more hidden layers, because testing of one province takes over one week or even longer in current structure of the MATLAB script.

L233: This is nit-picky, but I always get confused if “to 2019” means the product runs through 2019 or ends in December 2018. I would consider either changing to “through 2019” or being specific and putting months in as well.

Response: Thank you for the suggestion. The specific months was added.

L237: This is great, I am glad the approach is gaining momentum. Could cite Gregor et al. (2019), that is the first place I have seen individual years used to improve independence.

Response: The citation has been added.

L253: Note that these datasets are not included in the SOCAT dataset since pco2 is estimated and not directly measured. It is important to note that this data is completely independent from SOCAT.

Response: Thank you for the suggestion. More description was added.

L297: consider changing “proved” to “provides evidence for”. I am not surprised SST and SSS are important since the solubility is a large driver of pCO2.

Response: The unproper description has been changed to “provides evidence for”.

L346: Make it clear this value is from your product

Response: Thank you for the suggestion. The description was modified as “The global open ocean average pCO₂ of the product generated in this work increased about 1.85 μ atm per year”.

L355: remove obviously

Response: The unproper description has been removed.

L434: Maybe “have similar spatial patterns with high pCO2 in the eastern equatorial Pacific” is a better way to phrase this.

Response: Thank you for the suggestion. The description was modified.

L474: I could not download the script or dataset. Please make sure these are available everywhere. Zenodo is a public repository to consider.

Response: The website was supposed to be globally available. I am not sure if the full stop of the last sentence was misleading. The website is <http://dx.doi.org/10.12157/iocas.2021.0022> without a dot at the end. If the download page is still not available in your region, we will use Zenodo as a second repository, because this work and the MSDC repository belongs to a same research program and the product is planned to be stored at the MSDC repository.

Typos

There may be more that I missed. Please read the manuscript carefully.

L41 : Surface

L60 : methods

L99 : pCO₂ and predictors

L175: store

L178: calculate

Response: Thank you for pointing out the typos. We noticed that in the manuscript the word “predictor” and “predicator” were totally confused. Now the typos were corrected.

Figures:

All the figures need more descriptive legends.

Fig. 1: This figure is very detailed. However, it's hard to identify where to start reading from and the legend is not detailed enough. For instance, the reader doesn't even know the difference between indicator pool and input pool from the figure alone and it is unclear what Endcheck and Eo represent. Consider either adding color to the diagram to make it easier to read or simplifying it.

Response: Thank you for the suggestion. More legends and descriptions were added in the figure.

Fig. 2: this is nice, a classic neural network diagram. However, add more details in the legend. To make it clear you could also add the equation below hidden layer and summation layer.

Response: The equation has been added in the figure.

Fig. 3: Consider naming the provinces something meaningful instead of numbers. For instance, East Equatorial Pacific, North Pacific Subpolar, North Pacific Subtropical, etc. I found myself constantly referring back to this image and names like this will make the paper easier to follow. Also, this looks similar to the Fay and McKinley biomes (<https://essd.copernicus.org/articles/6/273/2014/essd-6-273-2014.html>). I don't think this is necessary here, but I wonder if using 17 biomes could recreate the biomes?

Response: Thank you for the suggestion. The provinces name was changed to numbers following by locations. The Fay and McKinley biomes used SST, CHL-a and MLD, which are also used in this work. If using 17 biomes maybe the result will be more similar. But we want to use a simpler province set to make sure that there are as many SOCAT samples in each province, because the result of stepwise FFNN was largely influenced by the input SOCAT samples.

Fig. 4: this is fine, just add more description. Figure (a) could even be moved to supplementary.

Response: More description was added.

Fig. 5: Consider making the text larger on the colorbars. It is difficult to read.

Response: The figure was redrawn to make the colorbars larger.

Fig. 6: Consider moving this to supplementary. This figure doesn't add to the story.

Response: Thank you for the suggestion. The figure has been moved to supplementary.

Fig. 7: This is fine, the text could be larger, and consider removing the tick labels in the middle of the plot. I would also consider moving away from the rainbow colormap since it has abrupt color changes that are meaningless. Cmocean has nice colormaps and is available for python and matlab (<https://matplotlib.org/cmocean/>).

Response: Thank you for the suggestion. The size of text was adjusted and the "balance" colormap from the Cmocean was used.

Fig. 8: This is fine.

Fig. 9: Consider replacing "previous climatology product" with "Landschützer et al. (2020) product" Also consider using a non-rainbow colormap. My suggestion is the thermal colormap in cmocean.

Response: Thank you for the suggestion. The title has been replaced. The thermal colormap in cmocean was used.

Tables:

Table 1,2: these are nice, just more description.

Response: More description was added.

Table 3: Consider changing the province names to something more descriptive so the reader doesn't have to constantly refer back to the figure.

Response: Thank you for the suggestion. The province names were changed to description of spatial locations.

Table 4: Make the lowest MAE and RMSE for each province stand out. Bold those values or shade the box. This will allow you to quickly see which FFNN performs best in each province

Response: Thank you for the suggestion. The values were highlighted in bold.