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Reply on RC3

Guorong Zhong et al.

Author comment on "Reconstruction of global surface ocean pCO_2 using region-specific predictors based on a stepwise FFNN regression algorithm" by Guorong Zhong et al., Biogeosciences Discuss., https://doi.org/10.5194/bg-2021-224-AC3, 2021

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 CO_2 flux estimated by sea-air pCO_2 differences using different pCO_2 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 pCO_2 differences by piston velocity, seawater density and CO_2 solubility, based on pCO_2 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 fCO_2 and pCO_2 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 (m^3 mol^{-1}) and δ (m^3 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 pCO_2 products, and some predictors were first used in the pCO_2 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 supplementary, 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 predicators with the result using same predicators in all provinces. more obvious border lines appeared in some regions when using different predicators in each province, but we are not sure whether it is caused by application of a certain predicator or by the differences of predictors between neighboring provinces.

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

Response: We extended the boundaries of all provinces 5 1°×1° grids width outside. In each one province, samples near the province boundary but belong to other province were also involved in the training process. For example, if province P1 and P2 are neighboring, samples belong to province P2 near the boundary of P1 were also used in the training of FFNN of P1. The distribution of pCO2 became smoother after this definition of province boundary was used.

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, predicators of pCO_2 are going to be added and removed one by one, and which predicators will be finally used in the pCO_2 predicting is determined according to the real-time change of predicating 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.

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 pCO_2 of the product generated in this work increased about 1.85 µatm 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.

References mentioned in this review

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Please also note the supplement to this comment:
https://bg.copernicus.org/preprints/bg-2021-224/bg-2021-224-AC3-supplement.pdf