

This manuscript uses a stepwise feed-forward neural network (FFNN) to identify an optimal feature for the prediction of ocean pCO<sub>2</sub>. The authors first use a self-organizing map (SOM) to cluster the ocean into 12 provinces based 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 pCO<sub>2</sub> 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.

**Below are specific line comments.**

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

L41 : I would consider rephrasing the “Surface ocean pCO<sub>2</sub> is ...” sentence to something like “The magnitude and direction of the flux is largely set by the air-sea pCO<sub>2</sub> 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.

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 pCO<sub>2</sub>:

SST and SSS --> solubility  
Chl-a --> phytoplankton uptake  
MLD --> entrainment  
xCO<sub>2</sub> --> Henry's law

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

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.

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

L102 : I like that you included units for the gas constant, please include units for each term (pCO<sub>2</sub>, fCO<sub>2</sub>, P, etc.)

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 pCO<sub>2</sub> products.”

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

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

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

L135 : Why were 12 provinces chosen?

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.

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

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.

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

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

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.

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

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

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

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.

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.

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.

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 pCO<sub>2</sub>.

L346: Make it clear this value is from your product

L355: remove obviously

L434: Maybe “have similar spatial patterns with high pCO<sub>2</sub> in the eastern equatorial Pacific” is a better way to phrase this.

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

## **Typos**

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

L41 : Surface

L60 : methods

L99 : pCO<sub>2</sub> and predictors

L175: store

L178: calculate

## **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.

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.

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?

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

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

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

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/>).

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.

### **Tables:**

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

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

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

### **References mentioned in this review**

Cheng L., K. Trenberth, J. Fasullo, T. Boyer, J. Abraham, J. Zhu, 2017: Improved estimates of ocean heat content from 1960 to 2015, *Science Advances*, 3, e1601545.  
<https://advances.sciencemag.org/content/3/3/e1601545>.

Fay, A. R., and G. A. McKinley. "Global open-ocean biomes: mean and temporal variability." *Earth System Science Data* 6.2 (2014): 273-284

Gregor, Luke, et al. "A comparative assessment of the uncertainties of global surface ocean CO<sub>2</sub> estimates using a machine-learning ensemble (CSIR-ML6 version 2019a)—have we hit the wall?." *Geoscientific Model Development* 12.12 (2019): 5113-5136.