Interactive comment on “A neural network-based estimate of the seasonal to inter-annual variability of the Atlantic Ocean carbon sink” by P. Landschützer et al.

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Landschützer et al. offer a new methodology for estimating the surface ocean pCO2 at monthly temporal and 1x1 spatial resolution for the period 1998 to 2007. They use a Self Organizing Map to identify biomes, and then within these biomes, they use a Neural Network to develop statistical relationships between pCO2 and predictor variables. These relationships are then used to estimate pCO2 in all points in space and time.

This paper presents the methodology of this approach, and discusses results for the Atlantic Ocean. Presumably a publication for the global results is in preparation. If so,
this paper will be referenced for the methodology. Thus clearly showing the methodology leads to robust results is important not only for this publication but for others likely to appear in the near future. Clarity is not sufficient in the current draft and needs to be significantly improved prior to final publication.

Major Comments

1. There are many parts to this analysis, and the reader needs to understand the robustness of the final product. The RMSE to the data that goes into the NN is not sufficient. A more rigorous approach of using only part of the data to train the SOM and NN, and then comparing the resulting predictions to actual data that has been reserved from the training is needed. In the NN description in the appendix, there is reference to a “validation data set”, but this is part of the NN methodology (as far as it is explained). Instead, I would like to see residuals (as in Figure 3) of 2006-2007 pCO2 to algorithms calculated with NN training only over the 1998-2005 period (or another reasonable choice of years). This would be a much better test of the results. What does an RMSE of 10 uatm really mean when the data to which you are comparing was used in the training of the NN?

2. The paper also lacks discussion of the sensitivity of the results to input choices. There are many SST products, many MLD products, for example.
   a. What happens to these results if other choices are made?
   b. What happens if you do not use the surface chlorophyll? This is quite important to justify as it limits the results to post-1998.
   c. What happens if you do not use the Takahashi pCO2 climatology in the biome definition?

3. The use of Takahashi pCO2 climatology in both biome definition and in the validation of results (Figure 8) is another significant concern. To what degree are your results influenced by the assumptions of the Takahashi pCO2 climatology?
4. Overall, there is a lack of clarity in presentation of the methodology. Some examples: the figures that intend to present validation are only discussed with a sentence or two, the appendices are not directly referred to, acronyms and other terms are not defined. More detail on this is given with the “minor comments” below.

Minor Comments

Page 1 Content: "was also increasing" Comment: Replace with "increased"

Page 3 Content: "Here, we overcome most of these limitations by presenting a new neural network-based approach, which determines the non-linear relationships between the surface ocean pCO2 observations and a set of independent observations to produce basin-wide sea surface maps of pCO2 on a monthly basis." Comment: This statement is over-confident. Please comment on the limitations of this method.

Page 4, Comment: Thank you for including the fco2 to pco2 equation, rather than just stating "we converted"

Page 4 Content: "For SST, we use the National Oceanic and Atmospheric Administration (NOAA) Optimum Interpolation (OI) sea surface temperature v.2 (Reynolds et al., 2002), for CHL the SeaWiFS mapped chlorophyll (SeaWiFSProject, http://oceancolor.gsfc.nasa.gov/cgi/l3), for MLD the mixed layer depth data from the Estimating the Circulation and Climate of the Ocean, Phase II (ECCO2) project (Menemenlis et al., 2008), for SSS the Simple Ocean Data Assimilation (SODA) sea surface salinity data (Carton and Giese, 2008) and for xCO2,atm the monthly atmospheric CO2 from GLOBALVIEW-CO2 (2011). Furthermore, the monthly pCO2 climatology of Takahashi et al. (2009) is used as an additional input parameter for defining the biogeochemical provinces. Due to their strongly skewed distribution, mixed layer depth (MLD) and chlorophyll a (CHL) were log-transformed before use as predictor values." Comment: Discussion of the sensitivity to these choices is needed somewhere in the text. In the work of my group, we have found significant sensitivity to choices such as the MLD climatology – for example, the choice of ECCO vs de Boyer MLD vs ARGO climatological MLD can
influence our biomes significantly. How do such choices impact these results?

Page 4 Comment: The use of the word "binned" might be reconsidered if it is really averaging up to a larger spatial scale. Unless you are including the original number of data points in further calculations, "binned" might be the wrong choice of word. "Averaged" should suffice.

Page 5 Content: "Input vectors with empty vector elements were removed from the datasets" Comment: Thus in regions of very little pco2 data, your fits will be much less robust. How is this dealt with, and how much impact does it have? The terminology here of “input vectors” and “targets” needs explanation.

Page 5 Content: "Where no chlorophyll a satellite data are available, due to cloud cover, we estimate the sea surface pCO2 only with the remaining input parameters." Comment: What percentage of the cases? How is this spatially biased? Does it impact results?

Page 5 Content: "We use a self-organizing map (SOM) method (Kohonen, 1987, 2001) to partition the global ocean into 16 regimes of similar patterns, i.e., biogeochemical provinces. The choice of 16 provinces represents a subjectively determined optimum between too many regions with too little data and a high degree of correlation between the provinces, and too few regions with a lot of data, but too high variance in the data. The monthly SST, log(MLD), SSS, and climatological pCO2 data of Takahashi et al. (2009) were used as input for the SOM(see Table 1). We chose not to include chlorophyll, i.e., log(CHL), due to missing values from cloud cover. Details on the SOM method can be found in the Appendix." Comments: A better description of how the SOM works is needed here, and also include reference to the relevant appendix. Included in here is the pco2 data as analyzed to a climatology by Takahashi et al. 2009. Thus, the comparison to these data in section 3 does not appear to be fair. You have already wrapped these data in. Please explain. These data are monthly resolution or greater. Are the provinces moving by month when used as input for the feed-forward
method?

Page 5 Content: "Despite their strong seasonal dynamics in space (Fig. 1a) and time (Fig. 1b), the estimated biogeochemical provinces exhibit a coherent large-scale behavior, reflecting the well known oceanic structures such as the gyres, the equatorial regions, and the high-latitude North Atlantic." Comment: There is inadequate discussion of the figures. Please guide the reader through the regions in figure 1a. Please explain the significance of figure 1b, which tells you that some pixels occupy as many as 9 regions over the course of the period. Few stay in the same one the whole time. Is this sensible or just statistical jibberish?

Page 5 Content: "As a second step we use a feed-forward network (FFN) method to reconstruct the non-linear relationship between our input variables and the target, i.e., pCO2, separately for each of the 16 biogeochemical provinces. The FFN method is a type of back-propagation network method that is capable of approximating any function with a finite number of discontinuities (Demuth et al., 2008). The established relationship is further used to predict the pCO2 for each point in time and space where no observations are available." Comment: Please also explain the FFN with some more detail here and also refer to the appendix explicitly.

Page 5 Content: "FINP" Comment: Define acronym prior to use.

Page 5 Content: "Due to the temporal and spatial variability of the regimes and the heterogeneous distribution of the pCO2 data, large differences exist in the number of observations within the different provinces." Comment: What are the implications of this heterogeneity? What is the sensitivity to these settings? These things need discussion in the main text.

Page 6, Lack of independent data outside the North Atlantic subtropics should be noted as a challenge for your validation.

Page 6, Please provide more text explanation for the residuals presented in Figure 3.
There are some large residuals, causing concern with respect to the very low estimated errors RMSE of 10 and bias of -.10). Is this analysis based on the raw or 1x1 monthly data? Are these the same data that went into the NN analysis?

Page 7 Content: "Given the overall small bias and the low RMSE between the two very different methods to interpolate the data, it appears that the long-term mean surface ocean pCO2 can be very robustly estimated from the available observations." Comment: Again, what is the impact of including the climatology in the definition of your biomes?

Page 8 Content: "To determine the drivers behind the seasonal cycles, we split the long-term mean seasonal cycle at each grid cell into a thermal and into a non-thermal component (Takahashi et al., 2002; Sarmiento and Gruber, 2006)." Comment: Which sst data is used? Please state the equation applied.

Page 8 Content: "seasonal cycles of the thermally and non-thermally driven partial pressures tend to cancel each other (Fig. 9), consistent with previous analyses (Takahashi et al., 2002; Sarmiento and Gruber, 2006)." Comment: Include in fig 9 plots of Takahashi climatology thermal and non-thermal cycles.

Page 9 Content: "–1 i.e., 1.80$\mu$atmyr versus 1.90$\mu$atmyr" Comment: Include uncertainty on these trends, and on all others discussed here, similarly for the interannual variability.

Page 9 Content: "1.46 $\mu$atmyr for the non-thermal component, while the thermal driven trend is on average 0.37$\mu$atmyr–1)." Comment: Again, need to quote uncertainty. Is the thermal trend distinguishable from 0?

Page 9 All trends calculated here are initiated in 1998, which follows a very strong ENSO event. Fay & McKinley 2013 indicate that this choice of start year influences pCO2 trends around the world’s oceans, presumably due to ENSO’s global influence. What happens if you shift your trend calculation to 1999 or to 2000? Presumably, there
would be significant change in the results.

Page 10 Content: "The most recent study by (McKinley et al., 2011) suggest the latter to be the case, but reported 50-yr trends in heat storage (Levitus et al., 2012) and interior ocean oxygen changes in the North Atlantic (Stendardo and Gruber, 2012) indicate that the North Atlantic and in particular its subpolar gyre has been subject to multi-decadal changes. " Comment: Variability can occur on mutlidecadal timescales. But you imply that this would be a "trend". What do you mean, specifically, by a long-term trend? If you mean the long-term response of the ocean to anthropogenic climate warming, please state so. If you mean something other than this, please state that clearly.

Page 10 Content: "−0.39±0.13PgCyr−1 in 2001 up to −0.56±0.18PgCyr−1" Comment: These are not formally distinguishable by any reasonable measure, given their uncertainty. You cannot quote them as evidence of interannual variability.

Page 11 Content: "would be beneficial to extend the study period to further investigate responses to climate modes such as the NAO and to investigate multi-decadal variabilities. Currently however, we are limited to 1997 since no basin-wide chlorophyll a measurements are available before and chlorophyll a is a simple, but important proxy representing the relation between biology and pCO2." Comment: How much more error do you get without chl in your method? Are you saying that you cannot get reasonable results without satellite chl? If so, please state more clearly.

Page 11 General comment on text – There is mixed terminology throughout the paper with regard to the strength of the sink/trends. "significant", "stronger", "slower increase", "lower undersaturation". More consistent verbiage would make the message more clear.

Page 11-14 Appendix general comment – The Appendix is quite difficult to follow. The lack of definition of many terms (e.g. Weight matrix, "winner", distance function) is a significant problem with making the methodology make sense. Please define terminol-
ogy, and otherwise carefully proofread to enhance clarity.

Page 12 Content: "As a consequence, the biogeochemical provinces follow the seasonal pattern of the pCO2 climatology, meaning that the seasonality of pCO2 at any given location will be mostly determined by the seasonal changes of the biogeochemical provinces and to a lesser degree by the seasonal cycle of the input data in the second state. " Comment: Again, you have imposed the pco2 climatology on your results. How, then, can you justify your comparison/validation in figure 8?

Page 19, Put your results all the way to right, and next to the RECCAP best estimate

Page 20, Figure 1a - If the provinces are changing boundaries please identify what year/month this map is for.

Page 20, Why in 2a , the NAC region is somewhat filled in, but in 2b there is a much larger blank area? Please explain.

Page 22, In 5b, and 5a, what is going on between Greenland and Iceland with very high pco2 and high efflux? Looks wrong. Why does the method allow this feature to be retained? Does it impact results?

Page 23, Presumably a zonal average. This needs to be stated in the caption. Ditto for following figures.

Page 25: Why are the green triangles not all on the black line? Doesn’t the black line come from the same data that the green triangles comes from, thus shouldn’t all the green triangles fall on the black line?

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