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Interactive comment on "Estimating temporal and spatial variation of ocean surface $p\mathrm{CO_2}$ in the North Pacific using a Self Organizing Map neural network technique" *by* S. Nakaoka et al.

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Comment: The authors are using Self-Organizing Maps to produce basinwide surface pCO2 maps for the North Pacific from VOS-line pCO2 measurements and remote sensing data of SST, SSS, Chl and MLD. The reconstructed pCO2 values are compared to pCO2 data of time-series stations and independent observations. Overall evaluation: The present manuscript is a very useful study which will be relevant for a broad scope of readers. It is well written and all details are explained thoroughly. I have only one major point of criticism that deals with the estimate of the overall RMS-error of the method. I believe that the presented estimate of 17.6 μatm is misleading and most

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likely too low. I am confident that the manuscript can be published after this issue is addressed. Major point: As far as I understand the authors the RMS-error of 17.6 μatm is based on a comparison between the in-situ pCO2 measurements used for the labeling process of the SOM and the pCO2 estimates of the SOM. If this is true, the validation was not done against independent data as the SOM contains (a lower dimensional representation of) this training data. The study by Friedrich and Oschlies [2009a, JGR] cited by the authors clearly showed that the true RMS-error must be expected to be much higher if a validation against training data is used.

Reply:

Dear reviewer #3,

We thank the reviewer for the positive overall evaluation and all the useful comments. As far as the reviewer's major point is concerned we provide the following explanation: As explained by Telszewski et al (2009), a study cited here by the referee (Friedrich and Oschlies (2009a)) derived the basin-wide monthly maps of pCO2 in the North Atlantic for 2005 from modeled pCO2sea distribution using the SOM approach (they call it KFM). These authors report the basin-wide RMSE of 21.1 μatm. Such a relatively high error results mainly from the employed SOM training procedure, which is fundamentally different to that suggested by the method's developer Tuevo Kohonen. In his extensive work (Kohonen 2001, 501pp) he specifically highlights the fact that the SOM is not an extrapolation technique and by its virtue can only be used to estimate values and relationships from within the training range. As described in Sections 2.1-2.3 we use seven years of the whole grid data (SST, MLD, CHL and SSS) to train the SOM. This way the SOM "sees" the relationships between the training parameters in every grid point in the North Pacific, with daily frequency for the seven years. This enables maximum SOM efficiency, regardless of the spatio-temporal cover of the in situ measurements used for labelling, and ensures that the SOM has been preconditioned with comprehensive, basin-wide training knowledge with regards to the relevant biogeochemical processes. Friedrich and Oschlies (2009a) decided to train the SOM only with values

(SST, CHL) collected along the VOS lines in 2005 (2005 VOS coverage metadata was used to extract the values from the model output). Such a small data set carries very limited training knowledge, despite the very successful data gathering campaign in the North Atlantic in 2005. Processes occurring in the vast extent of the basin are never sampled (and therefore not included in the training), and when they are sampled, it very often happens only a few times during the year (Friedrich and Oschlies, 2009a; their Fig. 2 for monthly cover and Fig. 6 for seasonal cover). It is not surprising at all that such trained SOM produces poor estimates for regions biogeochemically different than those sampled for the training data (their Fig. 6). Moreover their “along the lines” RMSE is very low (6.3 μatm) giving the impression (and in fact being their conclusion) that the RMSE calculated along the lines is almost an order of magnitude lower then that for the entire basin (21.1 μatm). This conclusion is completely misleading because they trained the network on a very limited number of training data and therefore the model only recreates the relationships “along the lines” and is pitifully wrong elsewhere. Based on reviewer’s comment we calculated the RMSE for the North Pacific subset of the SOCAT database. It turns out to be 20.2 μatm, a slightly higher estimate than that obtained for the labeling data. Again, coming back to the theory behind SOM, it is not surprising that the 2 values are not significantly different. SOM is not trained on the pCO2sea data and by the time the pCO2sea is introduced to the procedure the network is “rigid” in a sense that no adjustments to the mapping algorithm are made. Telszewski (PhD Thesis 2009) shows that even an unrealistically large labeling data set does not improve the error significantly. SOM depends heavily on training parameters and this is where one should focus in terms of reducing uncertainty.

Comment:Why are the data shown in Figure 8 only used to “facilitate a discussion about the temporal variations of pCO2”? These measurements could at least provide an idea of how well the method works for extrapolation to areas not covered by the training data measurements.

Reply: We agree. We added the RMSE compared with SOCAT database in section

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2.7.1 and one for time series locations in section 3.2. These two additional error estimates should be sufficient to assure the reader or the error that should be associated with SOM estimates presented in this study.

Comment:Furthermore an estimate of the overall RMS-error needs to include all possible sources of pCO2- mismapping of the method. For example, the remote sensing data are subject to uncertainties which can be quite large and which will affect the SOM-estimate (and the SOM formation process as well). For a first order evaluation of this effect the authors could add noise representative of the remote sensing uncertainties to the data used for the mapping process and compare the resulting pCO2 estimates to the untainted reconstructions. It could be done in a similar way for the training process.

Reply: We added the uncertainty of SST, CHL and SSS in section 2.2 as described in our response to Dr. Wanninkhof. These combined add to the overall error of the method, but at this stage we do not venture the assessment of their relative significance. The uncertainty in MLD is not known at the moment. As for the first order evaluation, it is part of a wider assessment of all sources of error and as we explained in our response to Dr. Wanninkhof, we will consider a separate study including sensitivity assessments and other uncertainty subjects of interest to the reader. We thank you for your suggestion.

Comment:I don't think it would compromise the value of the method if the study came up with a higher overall RMS-error but it would certainly add to its credibility if this RMS-error estimate would be based on a more realistic validation. As much as an RMS-error of around 20 μatm may sound small compared to the overall mean pCO2, Watson et al. [1991, Nature] stated that a bias of 1 μatm in the global ΔpCO2 would already result in about 0.2 Pg/yr uncertainty in the estimated ocean carbon uptake.

Reply: Our answer above plus we will change our claimed accuracy from 17.6 to a range of 17.6-20.2 μatm .

Minor points: Comment: Is the presented method more skillful than simply using the Takahashi climatology? The first guess of pCO2(x,y) would be to refer to Takahashi(x,y). This first guess can be refined -as the authors do it- by adding a $\Delta pCO2/\Delta t$ * (t-t(ref.)). Does the SOM method result in smaller RMS-errors compared to these two ”cheaper” methods?

Reply: Above all this method provides a dynamic picture of pCO2sea distribution rather than a static climatological snapshot. Gridded data behind this manuscript will be freely available and the users will have to assess its skilfulness. Monthly values at 0.25 degree resolution for 7 years might be much more useful and realistic for several applications than the climatological snapshot. There already exists a gridded SOCAT product that provides an alternative to the LDEO climatology. In our opinion it is too early to judge its skill but there is a strong need for a more dynamic estimate of pCO2sea distribution than the reviewer's first guess.

Comment:page 4578 / line 18: The authors might want to include a reference for ESTOC (e.g. Gonzalez-Davila et al. [2010, Biogeosciences]) and use a more recent reference for BATS (e.g. Bates [2012, Biogeosciences]).

Reply: We added these references as you suggested.

Comment:Discussion on the use of SSS page 4579 / line 18 page 4587 / line 2 + 23 page 4592 / line 10 SSS has already been successfully used by Friedrich et al. [2009b, JGR] to map basinwide pCO2 in the North Atlantic. They have also provided an explanation why it is such a skillful predictor for pCO2: “Surface water pCO2 is, besides its dependence on sea level pressure, a function of DIC, total alkalinity, SST and SSS. Because for any individual ocean basin total alkalinity can, to good accuracy, be estimated from SSS using a nonlinear empirical fit [e.g., Eden and Oschlies, 2006], ARGO SST and SSS data already provide substantial (though local) information about parameters that determine pCO2”

Reply: Thank you for your suggestion. We corrected the explanation.

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Comment:page 4585 / section 2.6 I agree with the authors on their treatment of Chl. However, it is a little awkward to say that the difference is "negligibly small" when there is a lack of coverage. At least we need to know what percentage of data coverage this statement is based on.

Reply: We added the percentage of data coverage and the difference as you suggested and rephrased the paragraph.

Comment:page 4587 / line 27... The authors might want to consider refining their method by using ΔpCO2(x,y)/Δt which could be obtained from the CMIP5 data. I included a figure of the deviation from the value of 1.76 μatm/yr used by the authors derived from the CESM1-BGC model.

Reply: Thank you for making the figure and sending it to us. We understand its importance of examining long-term pCO2sea trend. We hope we will find the way to refine our method in the future.

Comment:page 4593 / line 13: I do not understand what the sentence starting with "Even if ..." is supposed to tell us.

Reply: We deleted the sentence.

Comment:Figure 2b Just curios: How are unlabeled neurons treated?

Reply: In this study as in Telszewski et al (2009), we don't use unlabelled (empty) neurons to map pCO2sea.

Interactive comment on Biogeosciences Discuss., 10, 4575, 2013.