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Poster # 105

Neural Network Technique for Gap-Filling of Satellite Ocean Color Observations for Use in Numerical Ocean Modeling

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Motivation:

To develop gap-filled satellite ocean color fields for use in biogeochemical, ocean, and climate forecast models.

Abstract:

NOAA's focus on developing/improving operational coupled ocean-atmosphere modeling and ecological forecasting requires establishing a robust data stream for addressing bio-physical feedback mechanisms and global ocean coupled physical-biogeochemical modeling. Assimilating/integrating ocean color observations linking biological processes and upper-ocean dynamics is needed to initialize and constrain model evolution. Integrating/assimilating satellite ocean color fields (chlorophyll-a, Kd_{490}, Kd_{PAR}) into NOAA's operational ocean models requires scientifically consistent and robust techniques for addressing data gaps. One possible approach is a Neural Network (NN) gap-filling technique, linking ocean color variability, primarily driven by biological processes, with the physical processes of the upper ocean. A NN method for correlating satellite ocean color fields with other assimilated satellite and *in situ* observations : a) instigates fewer assimilation errors and b) reduces reliance on sparse *in situ* ocean color observations. Satellite-derived surface variables [sea-surface temperature (SST), sea-surface height (SSH) and sea-surface salinity (SSS) fields] and ARGO *in situ* gridded profiles of temperature and salinity are employed as signatures of upper-ocean dynamics. Ocean color fields from NOAA's operational Visible Imaging Infrared Radiometer Suite (VIIRS) are used, as well as NOAA SSH and SST fields and NASA Aquarius mission SSS fields. The NN technique is trained for two years (2012 and 2013) and tested on the remaining year (2014). Results are assessed using the root-mean-square error (RMSE) and cross-correlations between observed ocean color fields and NN output. To reduce the impact of noise in the input and ocean color datastreams, an ensemble of NN are constructed with with different weights.

Data:

- VIIRS chlorophyll-a (NASA), composited daily and interpolated from 9-km resolution to a 1-degree grid
- ARGO temperature and salinity profiles for the top 75m (International Pacific Research Center, Hawaii; Lebedev, *et al.*, 2010), gridded (1-degree resolution) monthly-means interpolated to daily values
- Daily satellite SSH (NOAA; Leuliette *et al.*, 2010), 0.5-degree resolution interpolated to a 1-degree grid
- Daily satellite SST (NOAA; Reynolds *et al.*, 2007), 0.25-degree interpolated to a 1-degree grid
- Aquarius composited daily SSS (NASA JPL-PO.DAAC, Aquarius User Guide, V3, 2014; also, Tang *et al.*, 2014), 1-degree resolution.

These observations are well documented and available, or soon to be available, in near-real time. All data (2012-2014) were interpolated to the same one-degree latitude-longitude grid and are available at daily temporal resolution.

Background: Neural Networks

Neural networks (NN) are very generic, accurate, and convenient mathematical models that emulate complicated nonlinear input/output relationships through statistical learning algorithms. NNs approximate the transfer functions (mappings) between a large number of possibly-interconnected inputs and multiple outputs, even for nonlinear and not-well-known relationships. Neural networks employ adaptive weights, tuned through training with past data sets, to provide robustness with respect to random noise and fault-tolerance. While neural network training is a complicated and time-consuming nonlinear optimization task, NN training needs to be done only once for a particular application and then repeatedly applied to new data, providing accurate and fast emulations. However, to retain the required accuracy, retraining may be required periodically. Neural networks are also well-suited for parallel and vector processing. NN can be applied to any problem that can be formulated as a mapping (input vector vs. output dependence). Mapping can be symbolically written as:

$$Y = M(X); \quad X \in \Re^n, Y \in \Re^m \tag{1}$$

where *M* denotes the mapping, *n* is the dimensionality of the input space (number of emulating NN inputs), and *m* is the dimensionality of the output space (number of emulating NN outputs). Multi-layer perceptrons (MLP) are a generic tool for approximating such mappings (Krasnopolsky, 2013). MLP NN analytical approximations use a family of functions like:

$$y_q = a_{q0} + \sum_{j=1}^{k} a_{qj} \cdot \phi(b_{j0} + \sum_{i=1}^{n} b_{ji} \cdot x_i); \quad q = 1, 2, \mathrm{K}, m \tag{2}$$

where x_i and y_q are components of the input and output vectors *X* and *Y*, respectively, *a* and *b* are NN weights, and

$$\phi(b_{j0} + \sum_{i=1}^{n} b_{ji} \cdot x_i)$$

is a "neuron". Equation (2) is also a mapping, which symbolically can be represented as Y = NN(X).

A data set is required to train, test, and validate NN (Eqn 2). To train NN, an error function, *E*, is created and minimized to find an optimal set of coefficients a_{ij} and b_{ij}.

$$E = \frac{1}{N} \sum_{i=1}^{N} [Y_i - NN(X_i)]^2 \tag{3}$$

All input and output data are observations, which have different levels of noise, thus, errors in NN simulated data (*e.g.*, the Chl-a data depicted in Figure 2) are a combination of all these noises plus the NN approximation error. Using the NN Jacobian (vector of derivatives of NN output over inputs), the partial levels of noise in observations and relative impact of inputs can be estimated; thus, the NN can be used as an indirect estimator of the level of noise in observations. To reduce the impact of noise and to calculate a stable NN Jacobian, multiple NN with different weights are constructed and the ensemble mean is compared with a single NN for different metrics (e.g., bias, variability, error and cross-correlation).

Ensemble Member Performance

Table 1. Performance of single NNs (ensemble members) and the ensemble mean on validation data set for Chl-a [grid points with Chl-a > 1 mg/m³ are removed to reduce the impact of noisy data].

Ensemble Member	RMSE (mg/m^3)	Cross-Correlation
1	0.110	0.722
2	0.093	0.766
3	0.097	0.757
4	0.097	0.757
5	0.094	0.758
6	0.094	0.758
Ensemble Mean	0.091	0.792

Table 1: The ensemble mean has higher cross-correlation between the NN output and the VIIRS observations and lower RMSE than any of the individual ensemble members. **The ensemble mean clearly outperforms all the individual ensemble members, which suggests that random noise may be contaminating the input and/or observation streams.**

Relative Impact of Inputs on NN Output

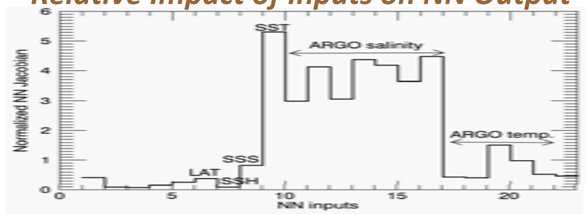

Figure 1: The linearized estimates (using NN Jacobian) of the contribution of various inputs — latitude, daily SSH, daily SSS, daily SST, monthly ARGO surface and subsurface temperature and salinity — on the ensemble NN output.

Figure 1 shows that **the most important input is the satellite SST, followed by the surface and subsurface ARGO salinity observations**. The surface ARGO temperature and salinity observations are less important than those from the subsurface, possibly because the satellite SST and SSS are able to capture some of the surface variability of temperature and salinity, respectively.

Bias

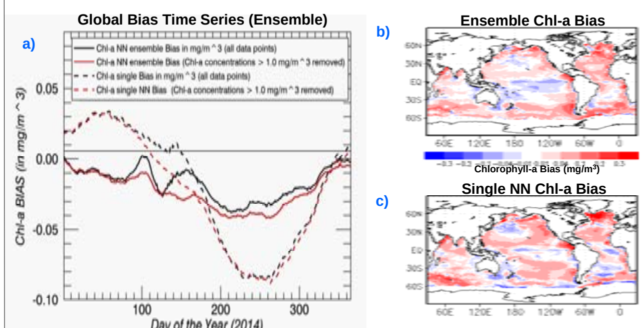

Figure 2: Neural network (NN) chlorophyll-a (chl-a) bias, referenced to VIIRS observations (NN – VIIRS values): a) global mean bias [full data set = black; chl-a values exceeding 1.0 mg/m³ removed = red; solid lines for ensemble mean, and dashed lines for single NN] ; and global bias (chl-a > 1mg/m³ removed) for b) ensemble mean and c) for single NN.

The mean bias shows a clear seasonal cycle for the global oceans, with positive values during the boreal winter and negative values during the austral winter. The spatial pattern of bias (Fig 2b) has positive values in the equatorial Pacific Ocean and negative values in the equatorial Indian Ocean. Large bias values are found at high latitudes and in shallow waters. Thus, the bias is reduced when points where chl-a > 1mg/m³ are removed.

Variability Ratios

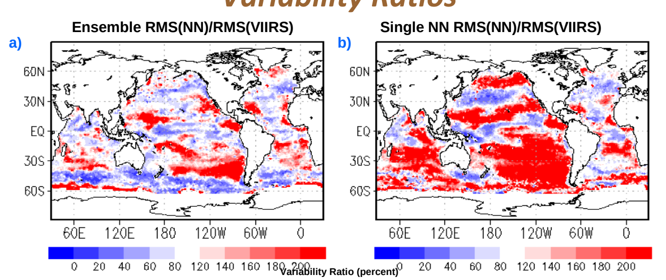

Figure 3: Percentage ratios of NN RMS Variability / VIIRS RMS Variability in percent for a) ensemble and b) single NN for chlorophyll-a (grid points with chl-a > 1mg/m³ removed).

Figure 3 depicts the ensemble NN's success in capturing chlorophyll-a variability in the VIIRS observations. The single NN estimates are over energetic with respect to VIIRS observations, while the ensemble mean has approximately the same level of variability as the VIIRS observations.

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Cross-Correlation

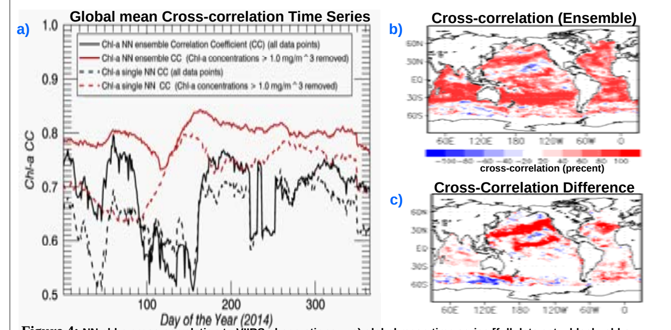

Figure 4: NN chl-a cross-correlation to VIIRS observations. a) global mean time series [full data set = black; chl-a values exceeding 1.0 mg/m³ removed = red; solid lines for ensemble mean and dashed lines for single NN] ; b) global ensemble mean cross-correlation (chl-a > 1mg/m³ removed); and c) cross-correlation difference between ensemble mean and single NN.

The cross-correlation (CC) is relatively high throughout the validation period (> 0.8), which is reassuring. The CC is more variable for the case where all data points are retained, suggesting that data points with chl-a > 1 mg/m³ are responsible for notably degrading NN performance. The NN has difficulty in certain regions, possibly because high spatial gradients and temporal variability in VIIRS chl-a values are not adequately sampled, currently, by the inputs (SST, SSS, T and S). The ensemble mean has higher CC than a single NN in the mid-latitude north Pacific and Atlantic oceans.

Error

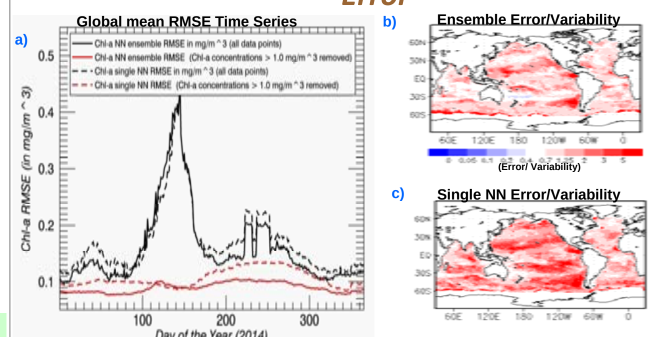

Figure 5: NN chl-a RMSE, referenced to VIIRS observations: a) global mean RMSE [full data set = black; chl-a values exceeding 1.0 mg/m³ removed (less than 1% of data removed) = red; solid lines for ensemble mean and dashed lines for single NN] ; and global bias (chl-a > 1mg/m³ removed) for b) ensemble mean and c) for single NN.

Figure 5 indicates that the error-to-variability [RMSE(NN)/RMS(VIIRS)] ratio is lowest in the center of the major ocean gyres. The overall error is small (< 0.1 mg/m³) for most of the year for the ensemble means. However, the signal is also small, so the error to variability is low (< 0.4) only in the center of the major ocean gyres. The ensemble mean outperforms the single NN noticeably almost everywhere.

Summary and Conclusions

- The NN method:
  - Provides an accurate, computationally cheap method for filling gaps in satellite ocean color fields.
  - Accurately estimates the seasonal cycle and large-scale spatial patterns in the VIIRS chl-a fields.
  - Best reproduces VIIRS chl-a variability in the major ocean gyres in the mid-latitudes.
- The largest errors are found where the spatial scales of variability are small and the variability is large, e.g., continental shelves, coastal regions, marginal seas, etc.
  - Removing data points with chl-a > 1 (less than 1% of points) improves NN performance.
- The ensemble mean outperforms each of the ensemble members. Clearly, random noise must be contaminating the input and/or observation data streams.
- The daily SST is the most important input, closely followed by ARGO monthly sub-surface salinity profiles. The ARGO monthly temperature sub-surface signal moderately contributes to NN performance.

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