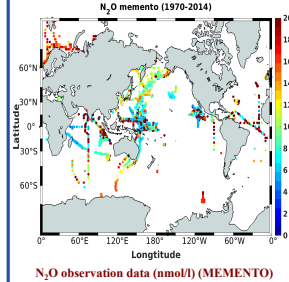




Motivation

- N₂O data in the various regions of the world ocean is rather sparse.
- Important to evaluate the impact of greenhouse gases on world climate.
- This motivates us to predict the spatial distribution of N₂O in the world ocean, based on other parameter values.
- Data driven machine learning models can be used to train the model for accurate estimation of N₂O concentration values.
- Predicted N₂O values can be used in other studies and research.



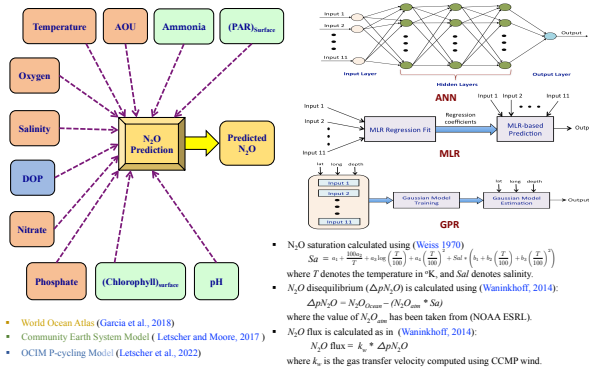
Objectives

- An attempt is made to simulate the global ocean N₂O distribution using the available database of N₂O observations.
- Carry out estimation of the global distribution of N₂O fluxes using well-sampled environmental variables.
- Use data-driven machine learning models to train the model.

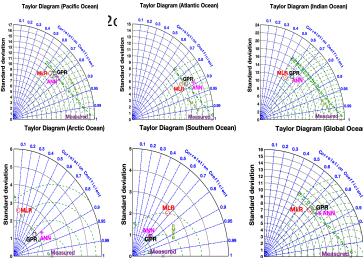
Research Approach

- We explore three alternate machine learning approaches for prediction:
 - Artificial Neural Networks (ANN): Mimics the behavior of brain.
 - Multiple Linear Regression (MLR): Deduces linear relationship among parameters.
 - Gaussian Process Regression (GPR): Based on Gaussian model training and estimation.
- In each approach, we first train the model using available datasets, and then predict the N₂O concentrations for the various ocean regions.
 - 70% of the available data are used for training.
 - 30% of the data are used to validate the quality of prediction.
 - The validated data are used to create an N₂O data product (3-D map) for the global oceans.
- For the ANN-based approach, 50 different network configurations are explored, and the average of the best 5 is used for the final prediction.

Dataset and Methodology

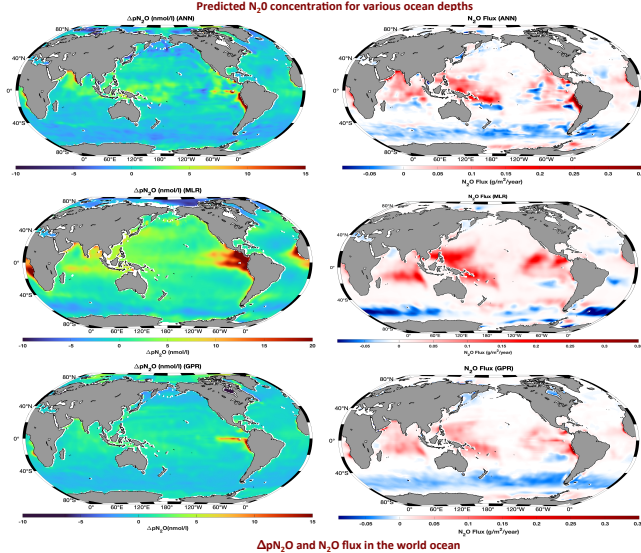
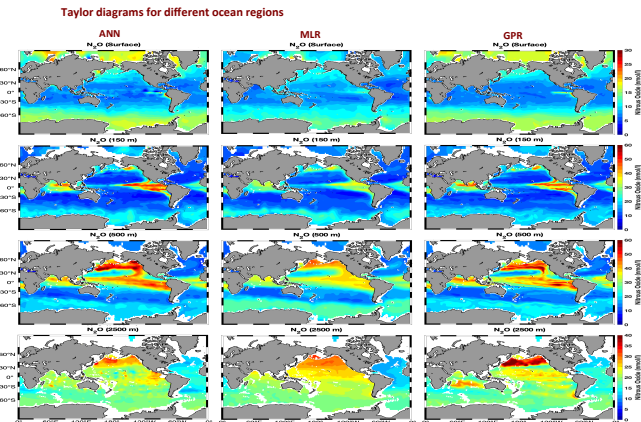


Results



Best five ANN configurations and prediction accuracy

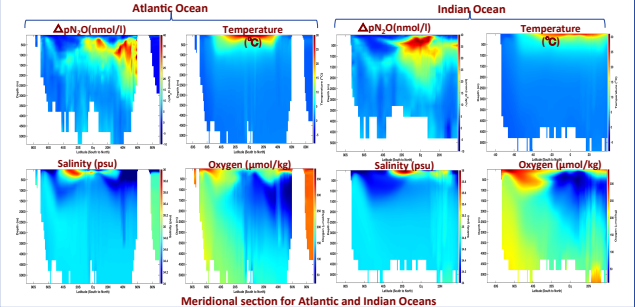
Sl. No.	ANN Configuration (No. of neurons in hidden layers)	RMSE (N ₂ O) (nmol/l)	CORR (N ₂ O) (Coefficient of correlation)
1	[90]	8.14	0.80
2	[100 85]	8.08	0.85
3	[100 95]	8.14	0.80
4	[95 90 80]	8.24	0.79
5	[100 95 90]	8.14	0.79



Results (contd.)

N₂O flux calculated using the three approaches

Region	Area (m ²)	Flux in Tg N yr ⁻¹		
		ANN-based	MLR-based	GPR-based
Pacific Ocean	6.38 × 10 ¹³	1.66 ± 0.106	1.85 ± 0.093	1.70 ± 0.105
Atlantic Ocean	3.99 × 10 ¹³	0.40 ± 0.049	0.77 ± 0.052	0.51 ± 0.038
Indian Ocean	4.25 × 10 ¹³	0.81 ± 0.224	0.53 ± 0.121	0.61 ± 0.152
Southern Ocean	0.77 × 10 ¹³	0.43 ± 0.007	0.35 ± 0.012	0.33 ± 0.004
Arctic Ocean	0.81 × 10 ¹³	0.33 ± 0.002	0.36 ± 0.006	0.32 ± 0.034
Global Ocean	3.17 × 10 ¹⁴	5.45 ± 0.094	4.57 ± 0.068	5.54 ± 0.074



Conclusions

- The machine learning models are found to perform satisfactorily, giving the best correlation of 0.85 and RMSE of ± 8.08 nmol/L.
- The ANN model is found to give better predictions for all regions except for Southern Ocean, where GPR model performs better.
- Depth profile across the global ocean reveals that maximum N₂O concentrations occur in the depth ranges of 250-1550 m (~26.2% of total) and 3300-4800 m respectively (~27.5% of total).
- We project a 5.45 ± 0.094, 4.57 ± 0.068 and 5.54 ± 0.074 Tg N₂O yr⁻¹ annual climatology of sea-to-air N₂O flux based on ANN, MLR, and GPR model predictions, which are within the range set by IPCC fifth assessment report (1.80-9.45 Tg N₂O yr⁻¹).
- Cooling of upwelled waters at Antarctic divergence create a net atmospheric N₂O sink.

Future Work

- Analysis of seasonal variability of N₂O flux using similar machine learning approach.
- Estimation of CH₄ flux using machine learning.
- Use N₂O data product to objectively calibrate dynamic cycling in CESM using inverse approach.

Acknowledgments

- U.S. Department of Energy. BER Award DE-SC0022177.
- CESM-BEC model output used for prediction. Source code is freely available at <http://www.cesm.ucar.edu/models/cesm1.2/>.
- Contact Dr. R. T. Letscher (UNH) for CESM-BEC output (Robert.Letscher@unh.edu).

References

- Garcia, H. E., Weathers, K., Paver, C. R., Smolyar, I., Boyer, T. P., Locarnini, R. A., et al. (2018). *World Ocean Atlas 2018, Volume 4: Dissolved inorganic nutrients (phosphate, nitrate and nitrite+nitrate, silicate)*. U.S. Dept. of Commerce.
- Letscher, R. T., & Moore, J. K. (2017). Modest net autotrophy in the oligotrophic ocean. *Global Biogeochemical Cycles*, 31, 699–708. <https://doi.org/10.1002/2016GB005503>.
- Letscher, R. T., Wang, W.-L., Liang, Z., & Knapp, A. N. (2022). Regionally variable contribution of dissolved organic phosphorus to marine annual net community production. *Global Biogeochemical Cycles*, 36(12), e2022GB007354. <https://doi.org/10.1029/2022GB007354>.
- Weiss, R. F., and B. A. Price (1980). Nitrous oxide solubility in water and seawater. *Mar. Chem.*, 8, 347–359.
- Wanninkhof, R. (2014). Relationship between wind speed and gas exchange over the ocean revisited. *Limnology and Oceanography: Methods*, 12(6), 351–362. <https://doi.org/10.4319/lom.2014.12.351>.