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BICEP
Biological Pump and Carbon Exchange Processes

DOC from space

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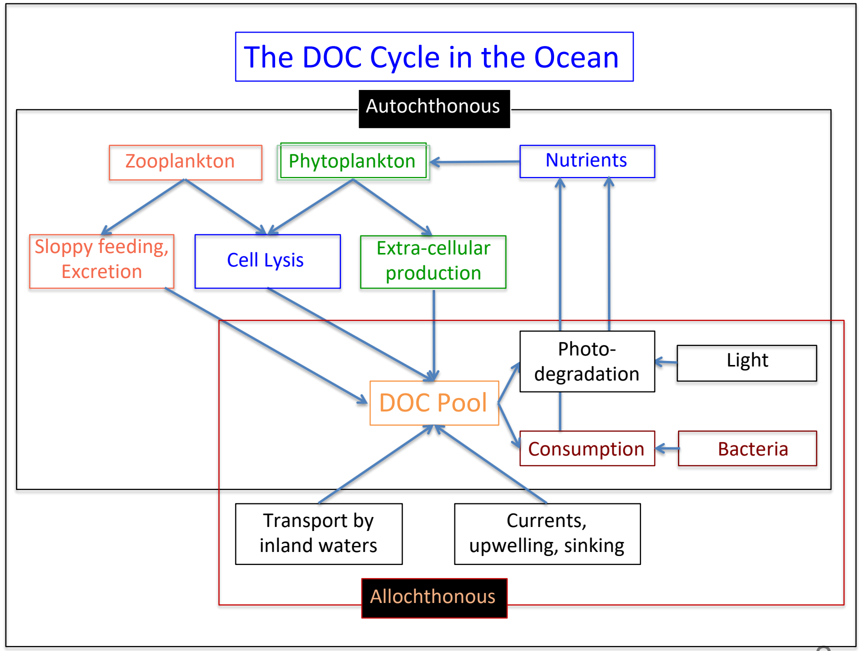
14.2.2022 **Ocean Carbon from Space Workshop**

Background

BICEP
Biological Pump and Carbon Exchange Processes

- ESA-BICEP project WP 3.4 Dissolved Organic Carbon.
- Use advanced non-linear statistical tools to elucidate the relationship between DOC and its satellite-based proxies.
- Here we concentrate on open sea DOC, using empirical approach with multiple satellite products.



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Data sets used in the analysis

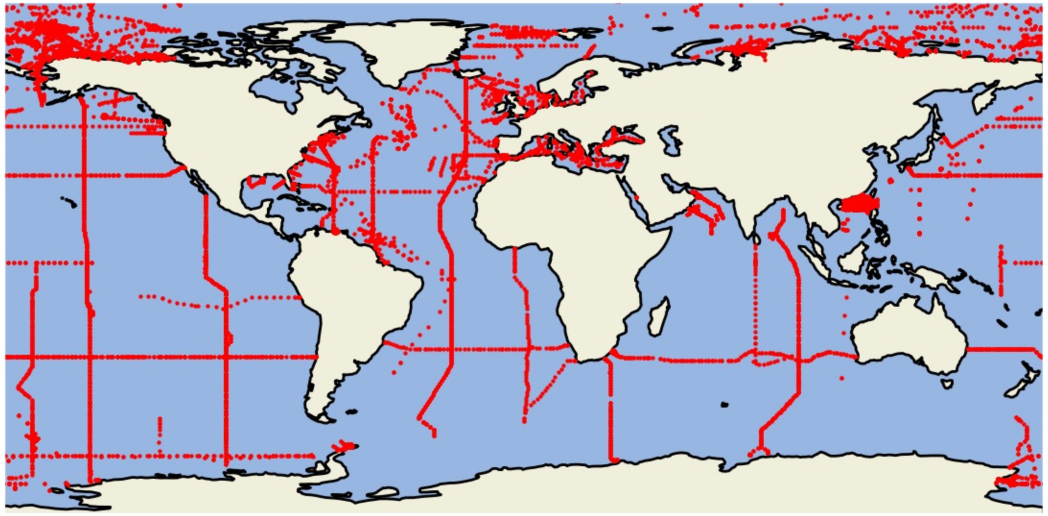
Data set	spatial resolution	temporal coverage	citation
Ocean Colour CCI	1/24°	1997–2019	Sathyendranath et al. [2019]
NPP	1/12°	1998–2018	Kulk et al. [2020]
Salinity CCI	1/12°	2010–2019	Boutin et al. [2020]
SST	1/25°	2007–2020	UK Met Office [2005]
in-situ		1994–2012	Aurin et al. [2018]
in-situ		1994–2020	Hansell et al. [2021]

Table 1: The data sets used. Except for the in-situ data, we are using monthly averaged data.

In-situ DOC data set by Hansel et al. 2021

- D. A. Hansell, et al.: Compilation of dissolved organic matter (DOM) data obtained from the global ocean surveys from 1994 to 2020, 2021. doi:10.25921/s4f4-ye35
- Merged with interpolated **monthly** Ocean Colour data and primary production.
- Total of 11200 DOC data points of which 8796 has OC and other regressor values.

In-situ DOC data locations



Different approaches to modelling DOC

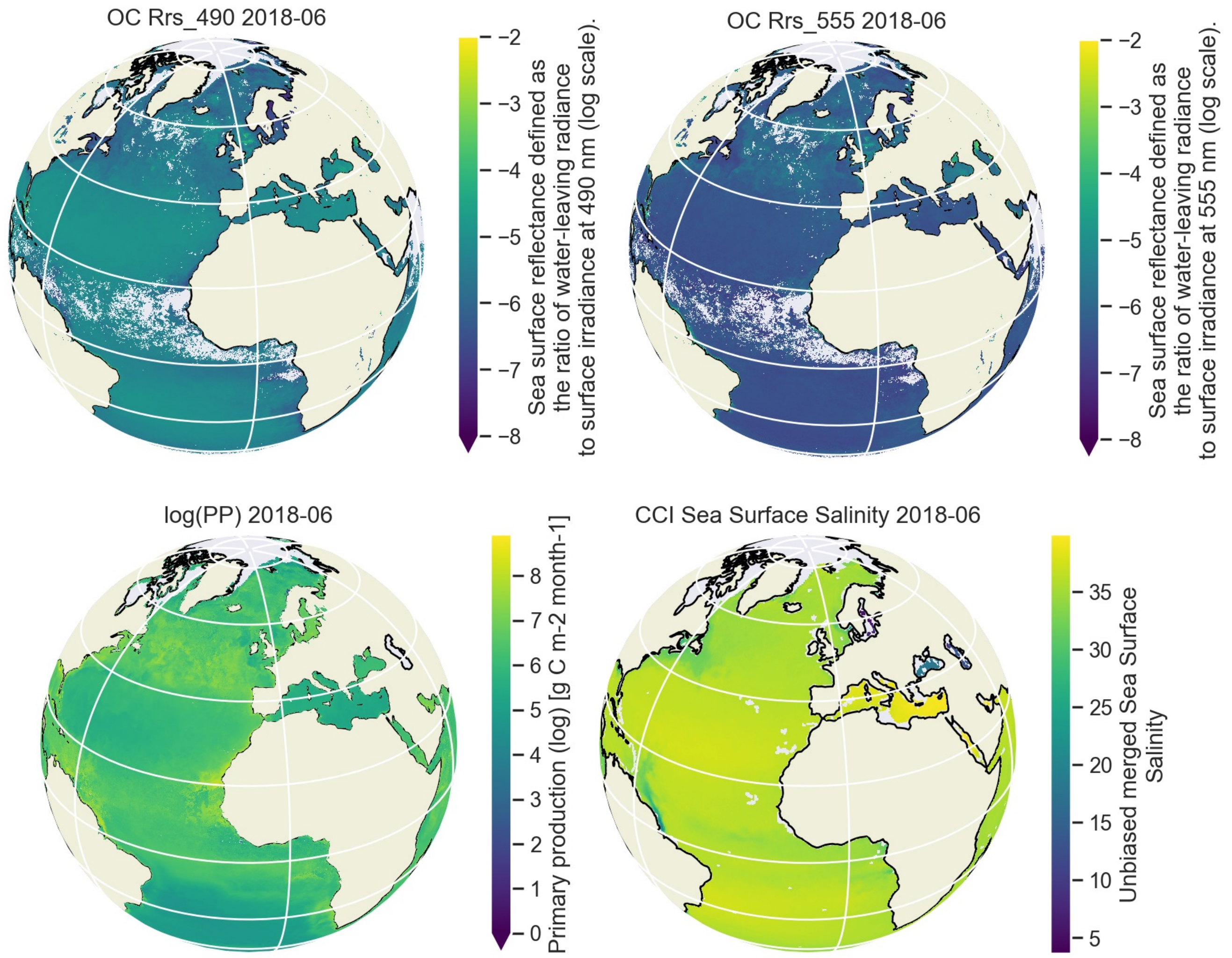
- Mechanistic/physical models (Hansel 2009, DeVries and Weber 2017).
- Statistical/empirical models (Mannino 2008, Hansel 2013, Aurin et al. 2018).
- Machine learning / AI (Aurin et al. 2018, Roshan and DeVries 2017).

- All are using more or less hybrid modelling, combining different approaches.

Empirical models for DOC using satellite based regressors

- Linear Regression.
- Neural Network.
- Gradient Boosting.
- Random Forest.

- DOC ~ Rrs_*nnn* + temp + salt + sqrt(pp) + lat + dts + depth + wclass



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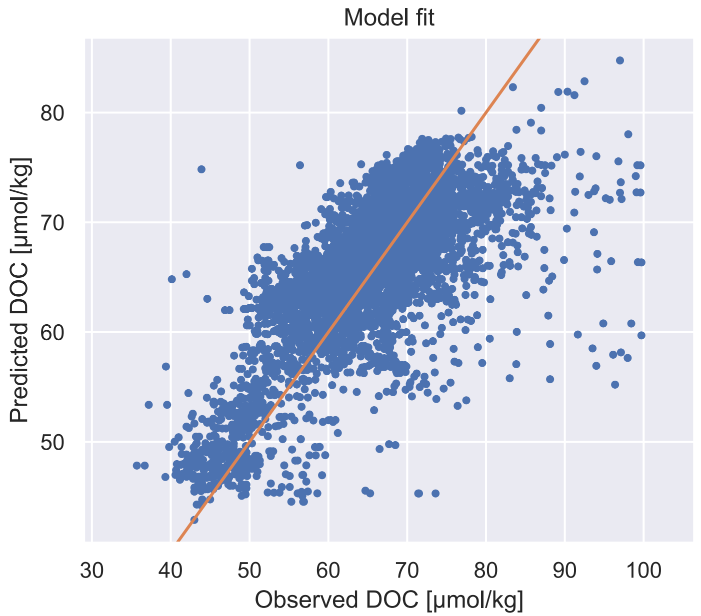
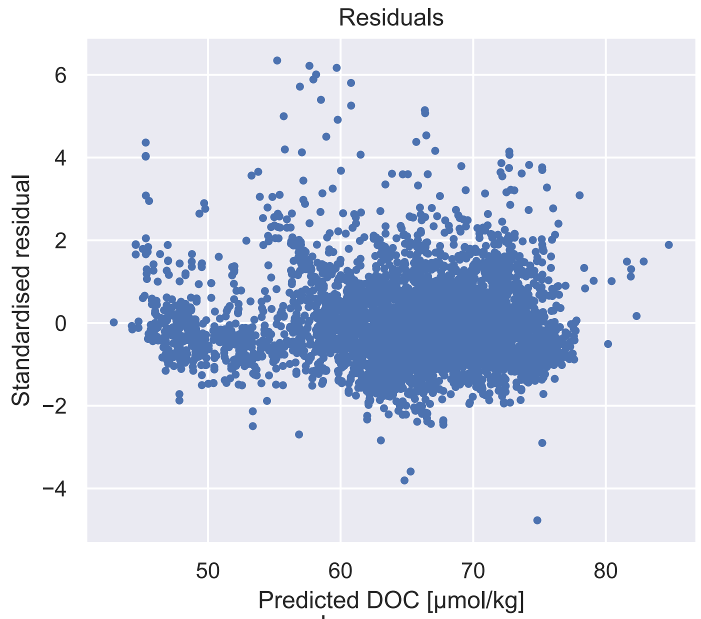
Kevin P. Murphy. Machine Learning A Probabilistic Perspective. The MIT Press, 2012.

Linear Regression

- Uses all Rrs variables, pp, salinity, temperature, latitude and distance to shore.
- R^2 = 53%.

Regression model output, > 300 km from shore, Hansel (2021) data set



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                            OLS Regression Results
==============================================================================
Dep. Variable:                    DOC   R-squared:                       0.529
Model:                            OLS   Adj. R-squared:                  0.528
Method:                 Least Squares   F-statistic:                     498.8
Date:                Fri, 11 Feb 2022   Prob (F-statistic):               0.00
Time:                        09:55:53   Log-Likelihood:                -16097.
No. Observations:                4897   AIC:                         3.222e+04
Df Residuals:                    4885   BIC:                         3.230e+04
Df Model:                          11
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept     63.3736      0.124    512.225      0.000      63.131      63.616
sqrtpp         0.8534      0.177      4.809      0.000       0.505       1.201
salt          -1.7989      0.187     -9.597      0.000      -2.166      -1.431
temp           8.1014      0.229     35.404      0.000       7.653       8.550
dts           -1.0577      0.115     -9.178      0.000      -1.284      -0.832
lat            1.5079      0.163      9.225      0.000       1.187       1.828
Rrs_412        1.4957      0.863      1.733      0.083      -0.196       3.188
Rrs_443        2.9970      1.173      2.555      0.011       0.697       5.297
Rrs_490       -3.4711      0.888     -3.911      0.000      -5.211      -1.731
Rrs_510       -1.1438      0.644     -1.775      0.076      -2.407       0.120
Rrs_555        1.6828      0.416      4.044      0.000       0.867       2.498
Rrs_670        0.4927      0.186      2.652      0.008       0.129       0.857
==============================================================================
Omnibus:                     1069.144   Durbin-Watson:                   0.485
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             3612.865
Skew:                           1.083   Prob(JB):                         0.00
Kurtosis:                       6.608   Cond. No.                         34.1
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
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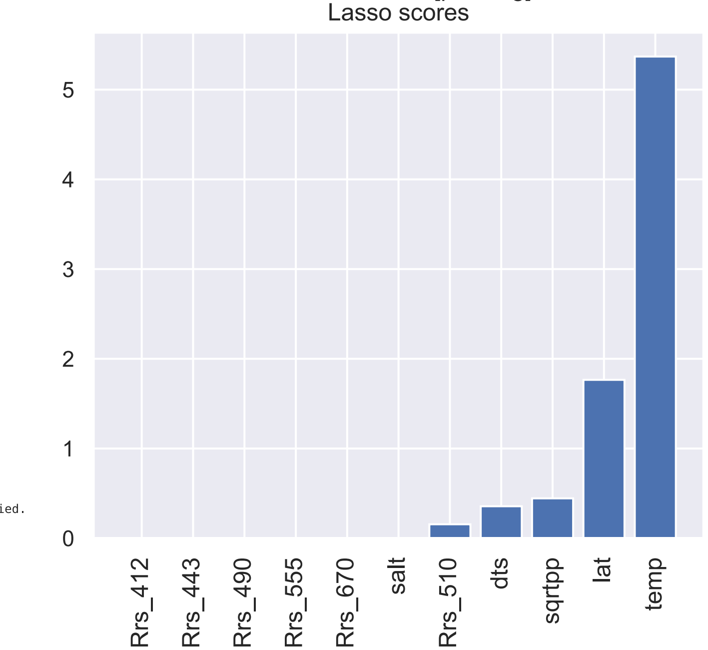
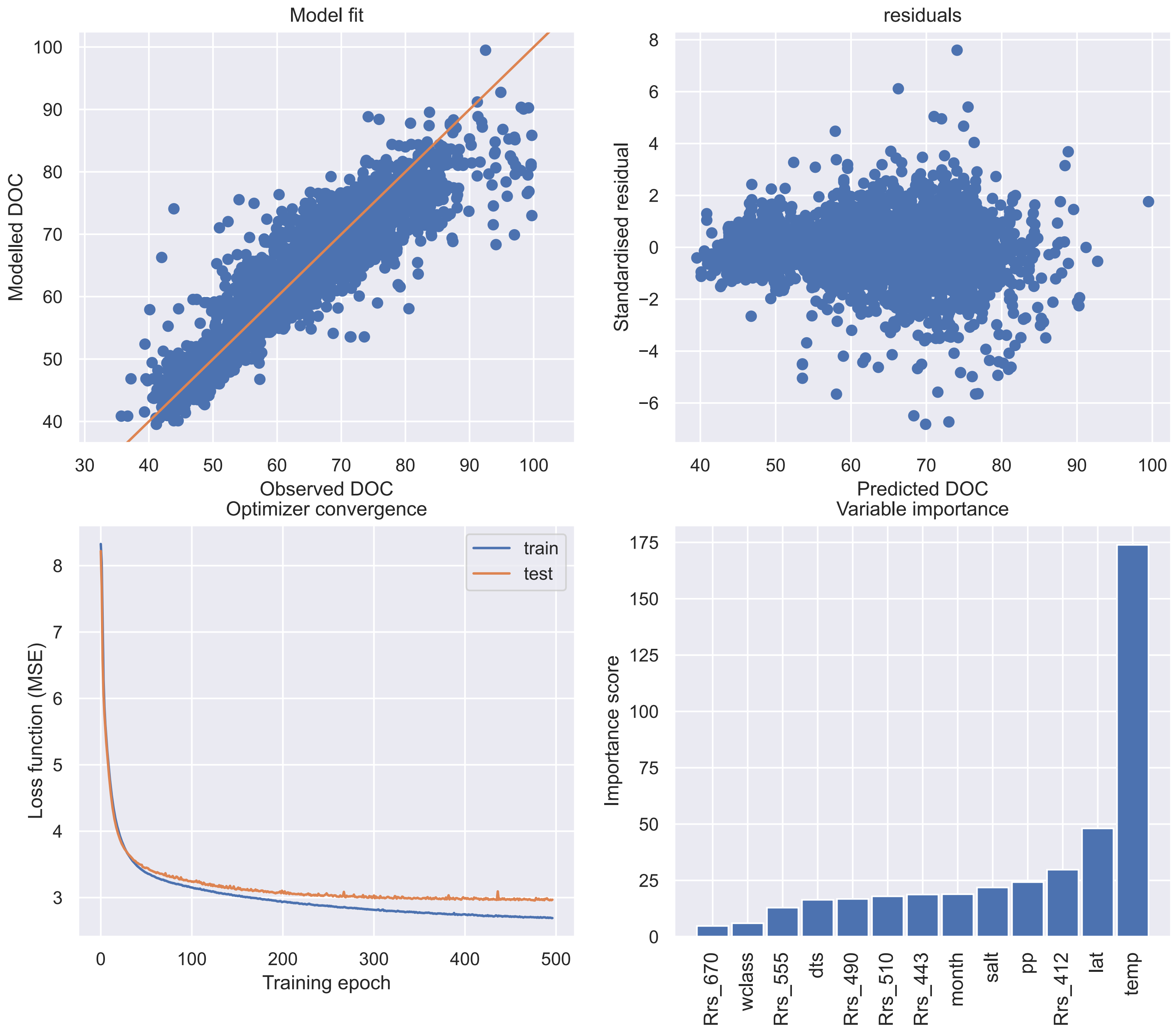


Neural Network

- Shallow net with one layer and 64 units.
- Uses water class and month as additional regressors.
- R^2: 80%

NN model output, > 300 km from shore, Hansel (2021) data set



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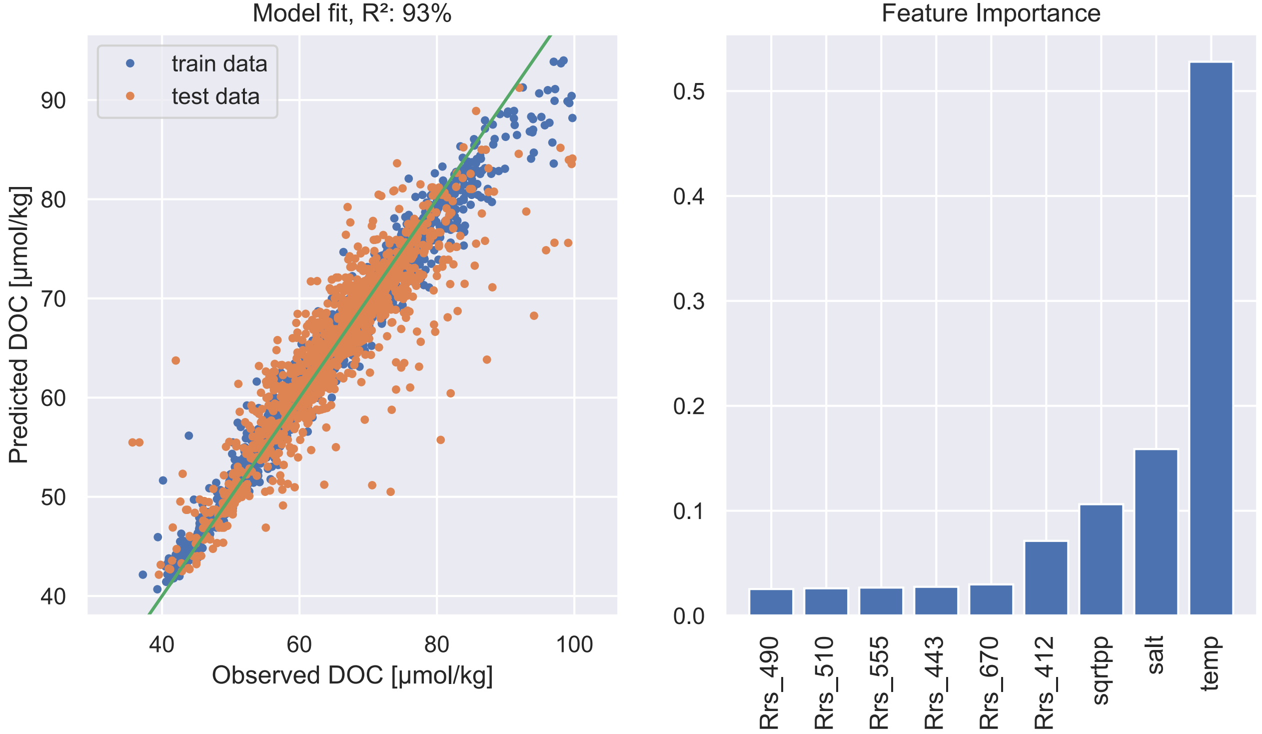
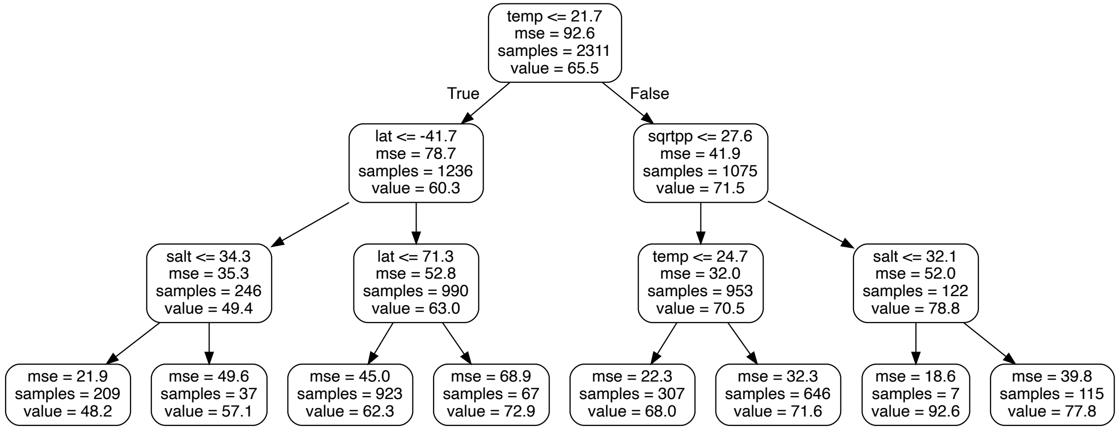
Random Forest Regression

- Best results for both train and test data sets.
- Used to produce global DOC data set.
- R^2: 94%

Random forest model output, > 300 km from the shore, Hansel (2021) data set





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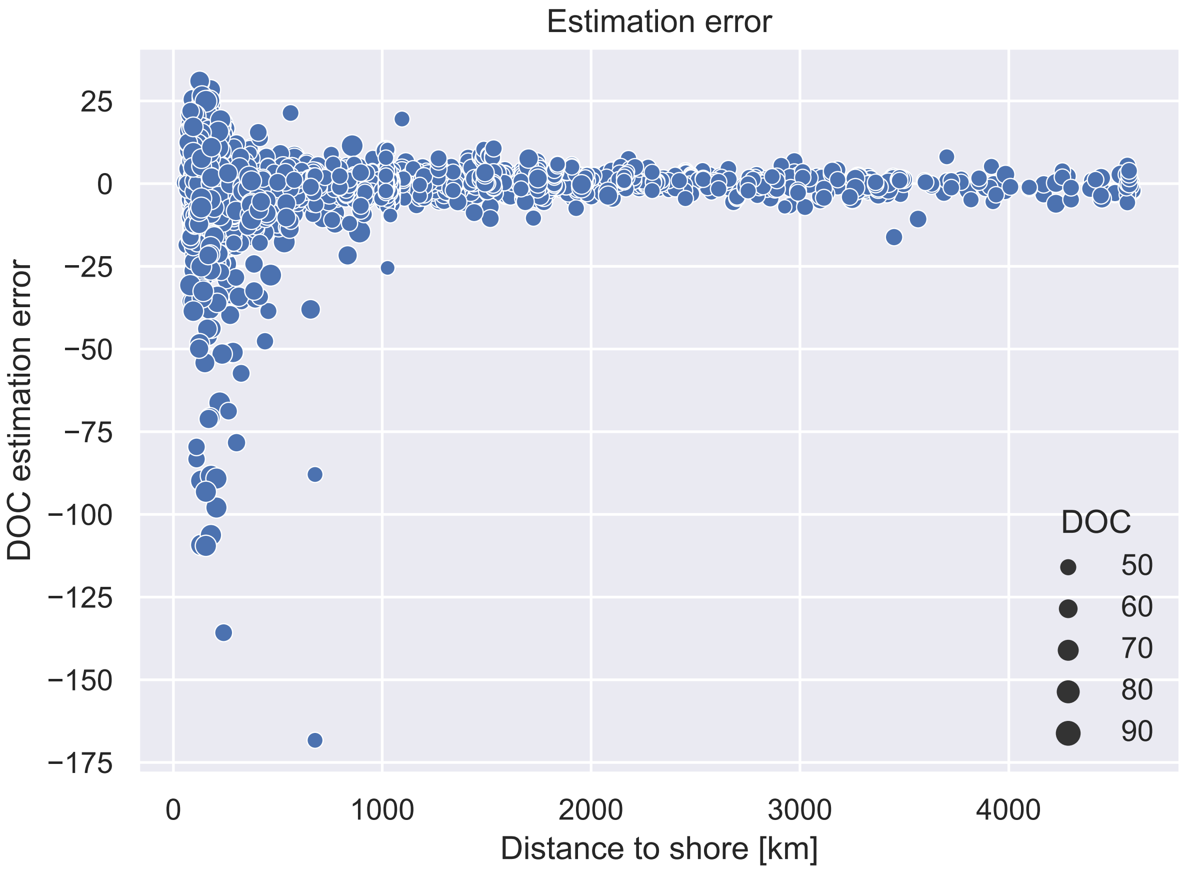
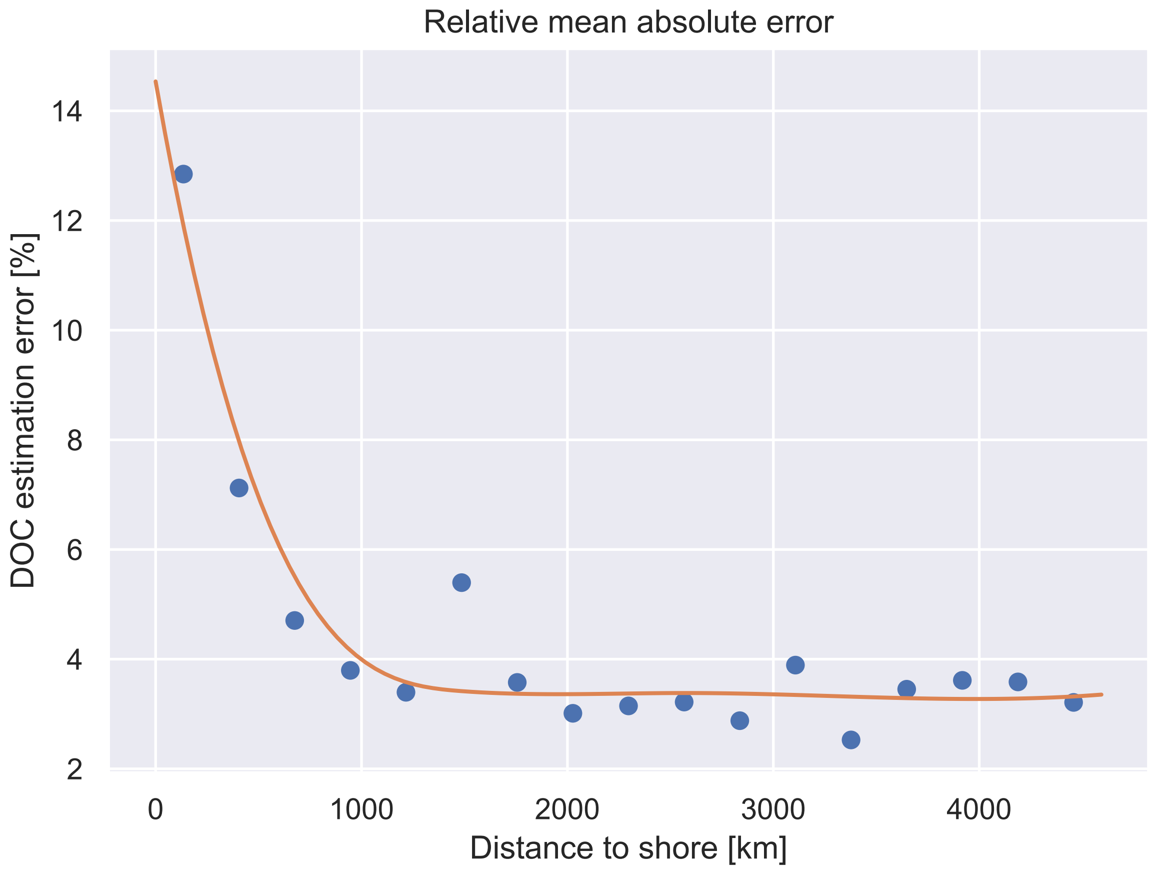
How to estimate uncertainty?





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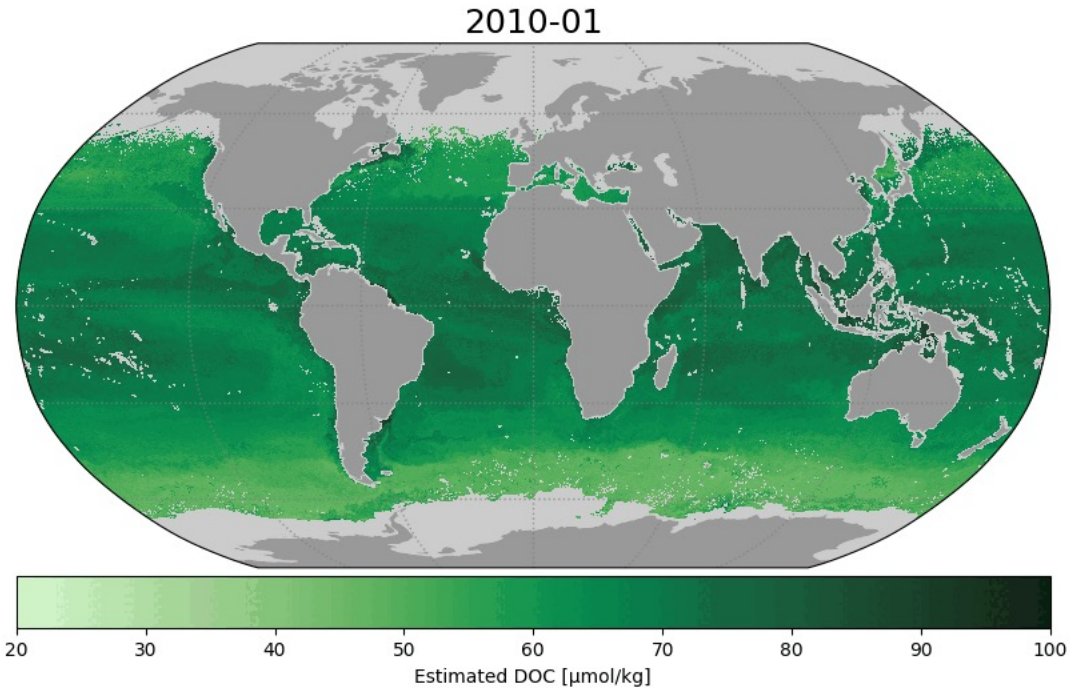
Estimated monthly DOC 2010-2018

- Generated using the Random Forest model.
- 1/12° spatial resolution.
- Monthly values for 2010-2018.

- Missing values are optionally interpolated linearly.



In-situ locations for each month shown as dots

Conclusions

- The new in-situ compilation by Hansel was used with Ocean Colour and other satellite based data.
- Random forest regression provided the best results.
- Proper uncertainty quantification and validation are still the challenges.
- A hybrid empirical–physical model would perhaps be the best option here.