

Revised Boosted Regression Tree Model

Based on reviewer comments we have revised our Boosted Regression Tree analysis (BRT) to create clearer and more detailed and interpretable results. Below we describe the revised steps and what changed compared to the previous version.

Data quality check

We have recalculated RCO₂P with an RQ of 0.9 for sites shallower than 50 m and an RQ of 0.85 for sites deeper than 50 m (Jørgensen et al., 2022) as opposed to RQ=0.9 for all sites in the previous version. We have also conducted a thorough review our data processing and have identified that two sites need to be omitted from data analysis as they do not meet the quality assessment of the resuspension assay method, i.e. the oxygen concentration decreased by >30% from before to after shaking (Bartl et al. 2025). We apologize for this mistake.

Multicollinearity

As common in ecological data sets, our variables display some collinearity which can be problematic for the interpretation of BRT results, particularly the ranking of individual feature importance, partial dependence plots and feature interactions (Boulesteix et al., 2012; Dormann et al., 2013; Elith et al., 2008; Lucas, 2020). Therefore, collinearity between all variables was checked using scatter plots and Pearson correlation coefficients (Figure 1). Mud content (Mud), medium sand content (M-Sand) and organic matter content (OM) showed strong multi-collinearity with correlation coefficients of $r = -0.91$ for Mud and M-Sand, $r = -0.84$ for OM and M-Sand, and $r = 0.89$ for Mud and OM. This suggest that these three variables contain very similar information and BRT models could be run with each of them interchangeably.

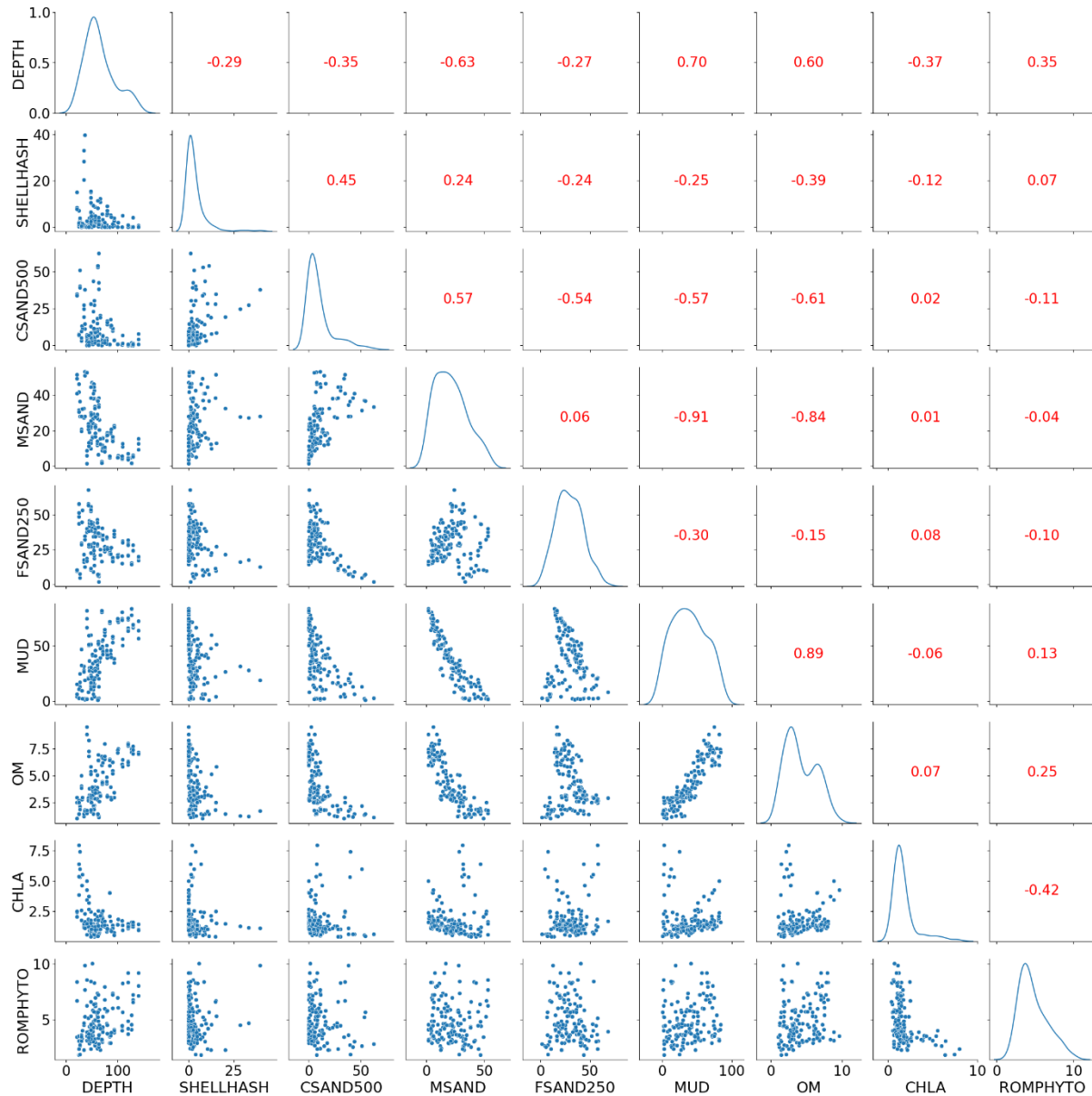


Figure 1: Scatter plots (bottom triangle), Pearson correlation coefficients (upper triangle) and data distribution (diagonal) of all environmental variables.

Revised BRT

We performed the BRT model with each of the collinear features (OM, Mud, M-Sand) individually, plus: water depth (Depth), shell hash content (Shellhash), content of coarse sands >500 μm (C-Sand), content of fine sand <250 μm (F-Sand), chlorophyll a content (Chl.a) and the ratio of organic matter to phytopigments (OM:Phyto).

We compare the BRT metrics and SHAP feature importances from our previous model with the revised BRT models (Table 1). The R^2 and RMSE are highly similar in all model-runs. In the revised BRTs, Mud, OM and M-Sand are by far the most important features, respectively. In all revised BRTs the 2nd to 4th feature are C-Sand, Depth, and F-Sand which shows that most of the RCO2P variability is explained by the same features in all models. Additionally, in the revised BRT with OM and the previous BRT, feature interaction importances (Fig. 2) and partial

dependence plots show the same patterns compared to the previous model (Figs. 3 and 4), which suggest that the corrections in the data set did not affect key relationships and patterns.

Table 1: Metrics of BRT model runs from original manuscript (previous BRT) and revised BRTs where one of the three collinear features was included. Presented are R^2 , root mean squared error (RMSE) and feature importance ranked based on mean absolute SHAP values (mean |SHAP|).

Metric	Previous BRT	Revised BRT with OM	Revised BRT with Mud	Revised BRT with M-sand
R^2	0.57 ± 0.1	0.57 ± 0.1	0.52 ± 0.1	0.56 ± 0.1
RMSE	0.56 ± 0.1	0.54 ± 0.07	0.57 ± 0.07	0.55 ± 0.09
Feature importance (mean SHAP)	1. OM = 0.42 2. Depth = 0.13 3. F-Sand = 0.12 4. M-Sand = 0.12 5. C-Sand = 0.12 6. OM:Phyto = 0.12	1. OM = 0.47 2. C-Sand = 0.15 3. Depth = 0.12 4. F-Sand = 0.1 5. OM:Phyto = 0.09 6. Chl.a = 0.07	1. Mud = 0.41 2. C-Sand = 0.19 3. F-Sand = 0.13 4. Depth = 0.1 5. Shellhash = 0.06 6. Chl.a = 0.06	1. M-Sand = 0.34 2. C-Sand = 0.15 3. Depth = 0.12 4. F-Sand = 0.07 5. Chl.a = 0.04 6. Shellhash = 0.04

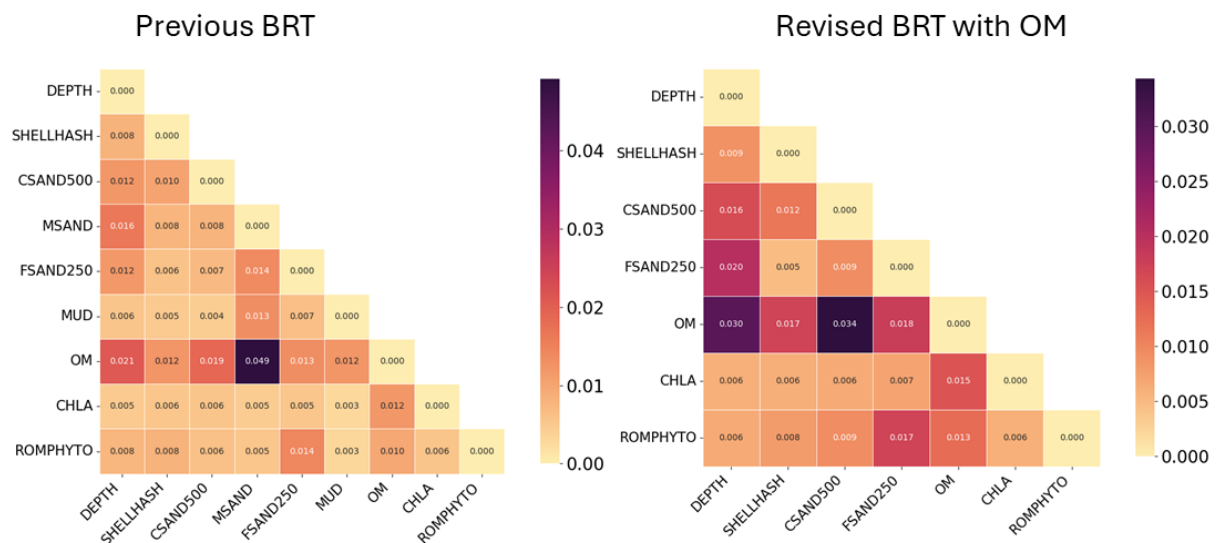


Figure 2: Heatmap of feature interaction importances of BRT model runs from original manuscript (previous BRT) and revised BRT with OM.

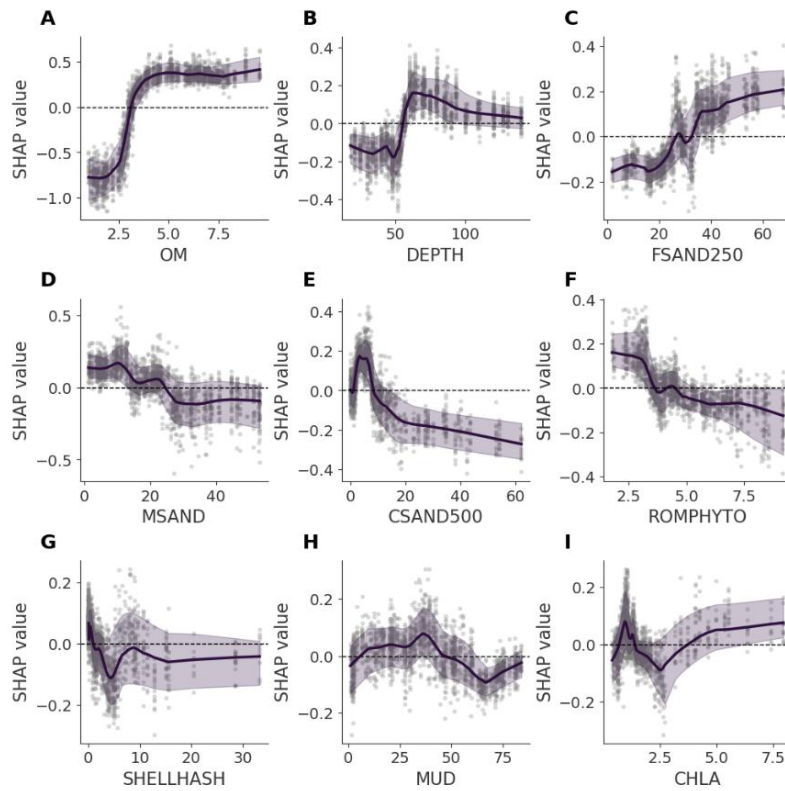


Figure 3: SHAP partial dependence plots of the BRT model from original manuscript (previous BRT). Graphs show the relationship between contribution to model output (modelled RCO2P) and individual features. Scatter shown for 50 model iterations, smoothed using LOWESS for mean, 90th percentile and 10th percentile.

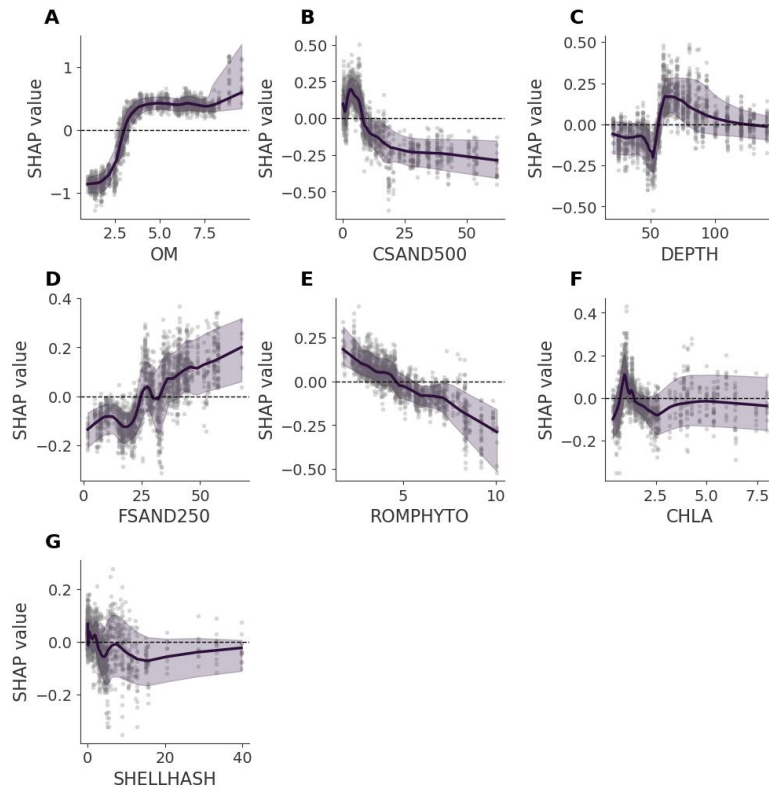


Figure 4: SHAP partial dependence plots of the revised BRT model with OM. Graphs show the relationship between contribution to model output (modelled RCO2P) and individual features. Scatter shown for 50 model iterations, smoothed using LOWESS for mean, 90th percentile and 10th percentile.

References

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