HOPB GPP model report

2023-01-30

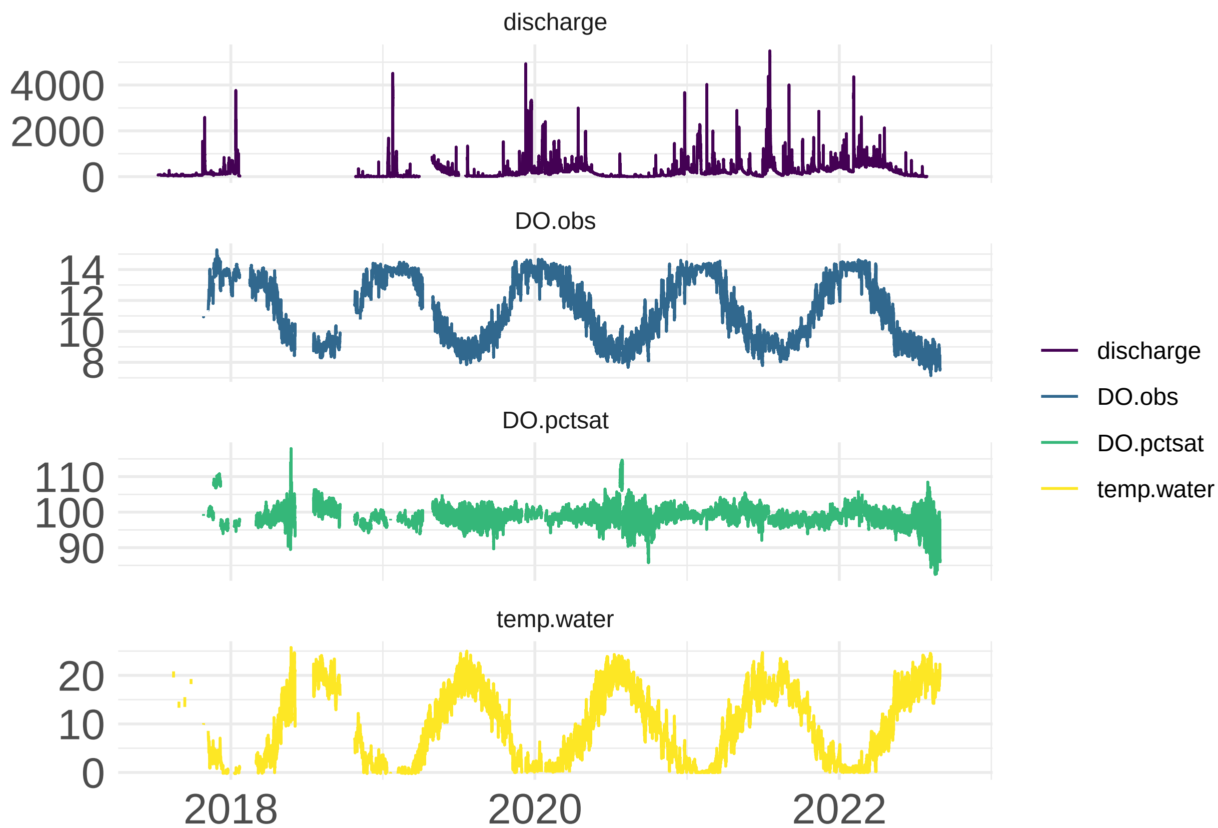


Figure 1: Full metabolism data streams.

The process for building a model suite and selecting a model is iterative. More details for data cleaning will be added here later.

We undergo a process to slim these models down based on a number of criteria. First, we throw out values that have very high estimates of GPP (> 1.5x maximum annual values observed in Berhnardt et al. 2022 Figure 1, ~5000 g C m^{-2} y^{-1}). Next, any models that have especially poor fits are excluded. In this case I automatically exclude any models that are in the upper 30% percentile of RMSE based on the model set, unless this is fewer than 5 models. This slimmed model set is the group I choose from after one final visual assessment.

I do a visual assessment of the slimmed model set to see how they compare and identify any days where the fit is especially poor across dates. To do this, I first chose the 'best' model of the set:

The 'best' model is: mm3_satq10

I then compute the model that is most different than the 'best' model and plot the metabolism estimates for each to visually assess.

Table 1: Full model output for all MLE models. 'modelID' represents the model identifier and also information regarding the assumed equations for GPPER. Unmodified models (e.g., 'mm1') represent the default 'mm_specs' of linear GPP̃light relationship. Saturating models (e.g., 'mm1sat') assume a saturating GPP̃light relationship. Lastly, Q10 models (e.g., 'mm1satq10') assume a saturating function of GPP̃light and an exponential function of GPP̃Temp. 'modelType' represents how daily K600 values are calculated, whether they are modeled simultaneously with GPP and ER (e.g., 'raw'), modeled as a function of daily discharge with varying relationships (e.g., 'loess', 'lm', 'mean'), modeled from observed night observation (e.g., 'night'), or from empirical gas release estimates (e.g., 'empiricalgam'). The empirical models are further identified by the model used to relate discharge to k, whether GAM or LM. 'RSME' represents the estimated relative root mean square error between observed and modeled dissolved oxygen concentrations standardized to the mean. 'negativeGPP' and 'positiveER' represent the number of days when daily estimates of GPP or ER are negative and positive, respectively. 'meanGPP' is the estimated mean GPP. This value can be scaled to different timeframes or units (i.e., carbon or oxygen) and must be check based on attributes of 'meanGPP'. 'maxK' is the maximum estimated daily k600 value.

modelID	modelType	RMSE	negativeGPP	positiveER	maxK	ER.Kcorr	meanGPP
mm1	raw	2.130000e+00	293	195	1.568945e+05	-0.985	7860.435
mm1_sat	raw	2.290000e+00	132	126	1.704003e+05	-0.980	5538.442
mm1_satq10	raw	1.970000e+00	121	107	2.818619e+04	0.539	4294.149
mm2	loess	2.010000e+00	269	138	5.146200e+01	-0.274	153.457
mm2_sat	loess	1.910000e+00	125	99	4.771600e+01	-0.069	192.650
mm2_satq10	loess	1.870000e+00	119	101	1.345211e+04	-0.411	752.218
mm3	lm	2.010000e+00	279	137	1.876520e+02	-0.100	137.747
mm3_sat	lm	1.890000e+00	120	105	5.698000e+01	0.075	186.377
mm3_satq10	lm	1.860000e+00	118	99	1.345211e+04	-0.411	744.053
mm4	mean	2.000000e+00	264	134	2.740900e+01	NA	120.336
mm4_sat	mean	1.860000e+00	122	105	3.237000e+01	NA	180.369
mm4_satq10	mean	1.880000e+00	116	100	1.345211e+04	-0.411	756.646
mm5	night	9.240818e+23	580	471	1.328860e+03	-0.945	36.893
mm5_sat	night	2.935628e+14	234	200	1.321886e+03	-0.999	38.148
mm5_satq10	night	1.882179e+23	216	186	1.122300e+03	-0.998	33.224
mm6	empirical-gam	4.040000e+01	223	120	1.316643e+10	0.021	869072.244
mm6_sat	empirical-gam	3.844000e+01	101	126	1.316643e+10	-0.189	36229.499
mm6_satq10	empirical-gam	4.995000e+01	137	129	1.316643e+10	-0.033	38334.026

[a] GPPmean = g C m-2 y-1

The most distant from best is: mm1_satq10

These plots are used to assess any dates that are especially bad (e.g., negative GPP, positive ER, very high GPP, etc.) across all models. This dates identified below for the 'top' model and are excluded from the analysis.

The most distant of the best models. Days between this model and above that are both bad are likely very difficult days to fit. Depending on how many of them there are we need to remove them or take a look at the QC flags or the timeseries data to decide if they should be thrown out.

The number of dates and proportion of bad dates within the best model are:

From here we assess any data removal and rerun until reasonably clean model outputs are achieved and a final model is chosen based on minimizing 'negativeGPP' and 'postiveER' and assessing the reasonableness of 'maxK'.

Lastly, we then take the top model suite and build an average model based on model fit, RMSE. To do so, we first remove models that have very high correlations between ER and K (i.e., $r \geq 0.80$) as these models are largely driven by variability in the estimates in K. Then we create a model weight based on relative model fit, *dRMSE*, the difference in relative root mean squared error from the best fitting model based on *RMSE* for a set of models, m, is:

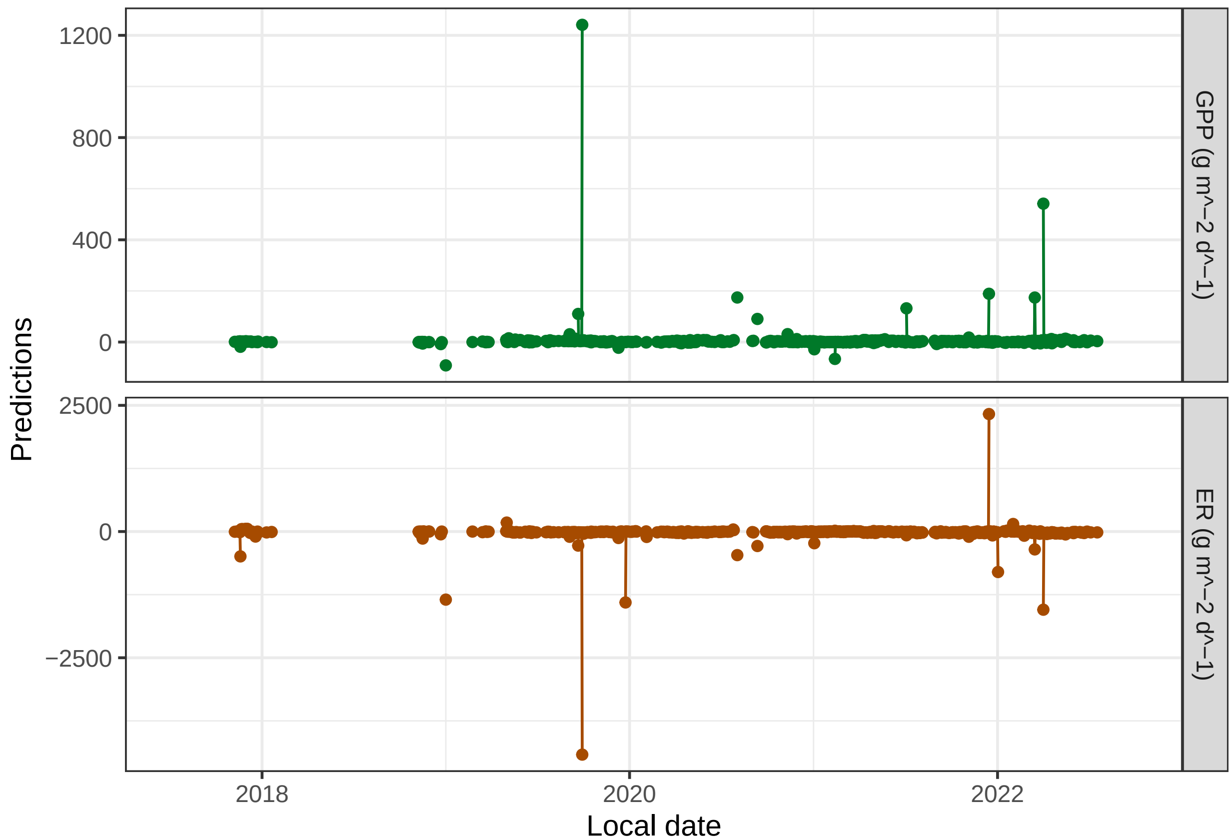


Figure 2: 'Best' model fit.

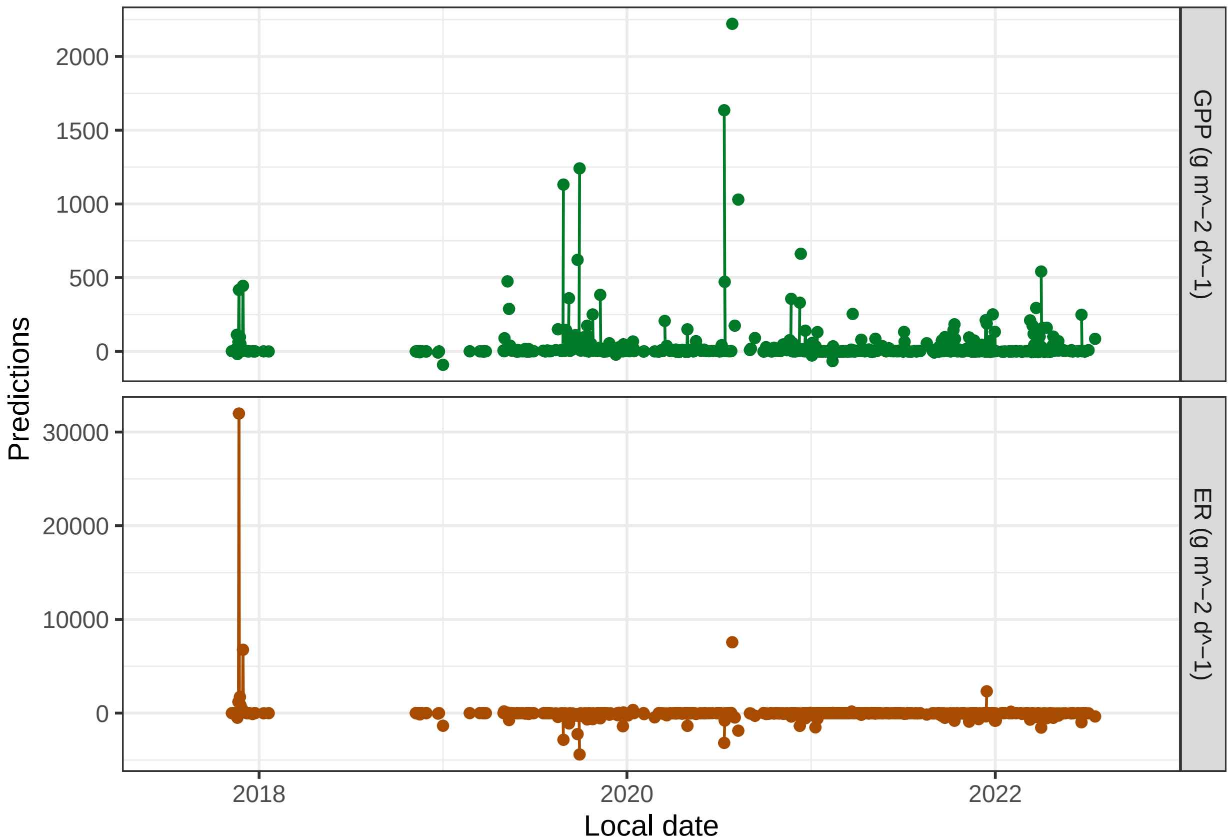


Figure 3: Most distant model.

Table 2: Slimmed model output for all MLE models. 'modelID' represents the model identifier and also information regarding the assumed equations for GPPER. Unmodified models (e.g., 'mm1') represent the default 'mm_specs' of linear GPP̃light relationship. Saturating models (e.g., 'mm1sat') assume a saturating GPPlight relationship. Lastly, Q10 models (e.g., 'mm1satq10') assume a saturating function of GPP̃light and an exponential function of GPPTemp. 'modelType' represents how daily K600 values are calculated, whether they are modeled simultaneously with GPP and ER (e.g., 'raw'), modeled as a function of daily discharge with varying relationships (e.g., 'loess', 'lm', 'mean'), modeled from observed night observation (e.g., 'night'), or from empirical gas release estimates (e.g., 'empirical-gam'). The empirical models are further identified by the model used to relate discharge to k, whether GAM or LM. 'RSME' represents the estimated relative root mean square error between observed and modeled dissolved oxygen concentrations standardized to the mean. 'negativeGPP' and 'positiveER' represent the number of days when daily estimates of GPP or ER are negative and positive, respectively. 'meanGPP' is the estimated mean GPP. This value can be scaled to different timeframes or units (i.e., carbon or oxygen) and must be check based on attributes of 'meanGPP'. 'maxK' is the maximum estimated daily k600 value.

modelID	modelType	RMSE	negativeGPP	positiveER	maxK	ER.Kcorr	meanGPP
mm1_satq10	raw	1.97	121	107	28186.187	0.539	4294.149
mm2	loess	2.01	269	138	51.462	-0.274	153.457
mm2_sat	loess	1.91	125	99	47.716	-0.069	192.650
mm2_satq10	loess	1.87	119	101	13452.114	-0.411	752.218
mm3	lm	2.01	279	137	187.652	-0.100	137.747
mm3_sat	lm	1.89	120	105	56.980	0.075	186.377
mm3_satq10	lm	1.86	118	99	13452.114	-0.411	744.053
mm4	mean	2.00	264	134	27.409	NA	120.336
mm4_sat	mean	1.86	122	105	32.370	NA	180.369
mm4_satq10	mean	1.88	116	100	13452.114	-0.411	756.646

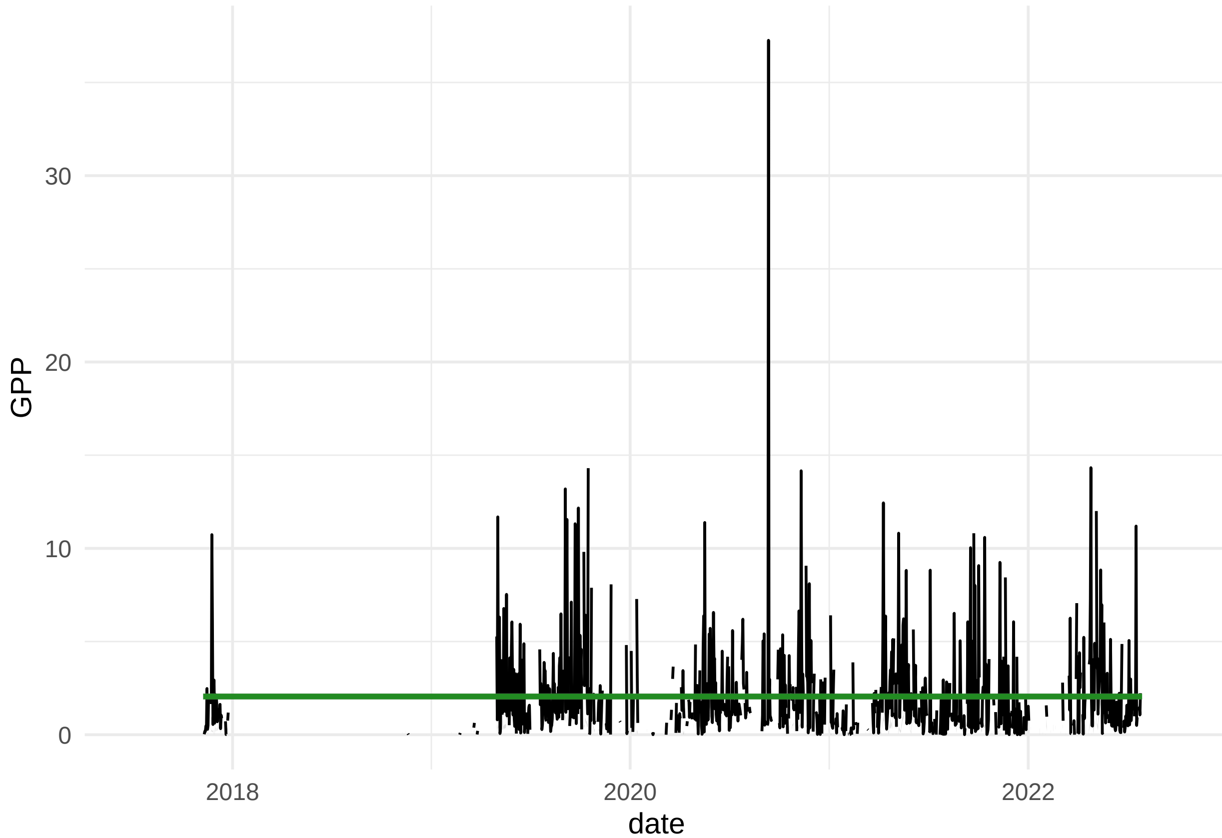
[a] GPPmean = g C m-2 y-1

lowGPP	lowGPPperc	highGPP	highGPPperc	NAs
216	20.93	16	1.55	2686

$$w_i = exp(\frac{1}{2}dRMSE_i)/\sum_{j=1}^{m} exp(\frac{1}{2}dRMSE_j)$$

From this, we create a weighted average model for GPP estimates, plotted below.

modelID	modelType	RMSE	negativeGPP	positiveER	maxK	ER.Kcorr	meanGPP	dRMSE	RMSEwt
mm1_satq10	raw	1.97	121	107	28186.187	0.539	4294.149	-0.11	0.098
mm2	loess	2.01	269	138	51.462	-0.274	153.457	-0.15	0.096
mm2_sat	loess	1.91	125	99	47.716	-0.069	192.650	-0.05	0.101
mm2_satq10	loess	1.87	119	101	13452.114	-0.411	752.218	-0.01	0.103
mm3	lm	2.01	279	137	187.652	-0.100	137.747	-0.15	0.096
mm3_sat	lm	1.89	120	105	56.980	0.075	186.377	-0.03	0.102
mm3_satq10	lm	1.86	118	99	13452.114	-0.411	744.053	0.00	0.103
mm4	mean	2.00	264	134	27.409	NA	120.336	-0.14	0.096
mm4_sat	mean	1.86	122	105	32.370	NA	180.369	0.00	0.103
mm4_satq10	mean	1.88	116	100	13452.114	-0.411	756.646	-0.02	0.102


30
20
10
0
GPP
2018
2020
2022
date