TECR GPP model report

2023-02-01

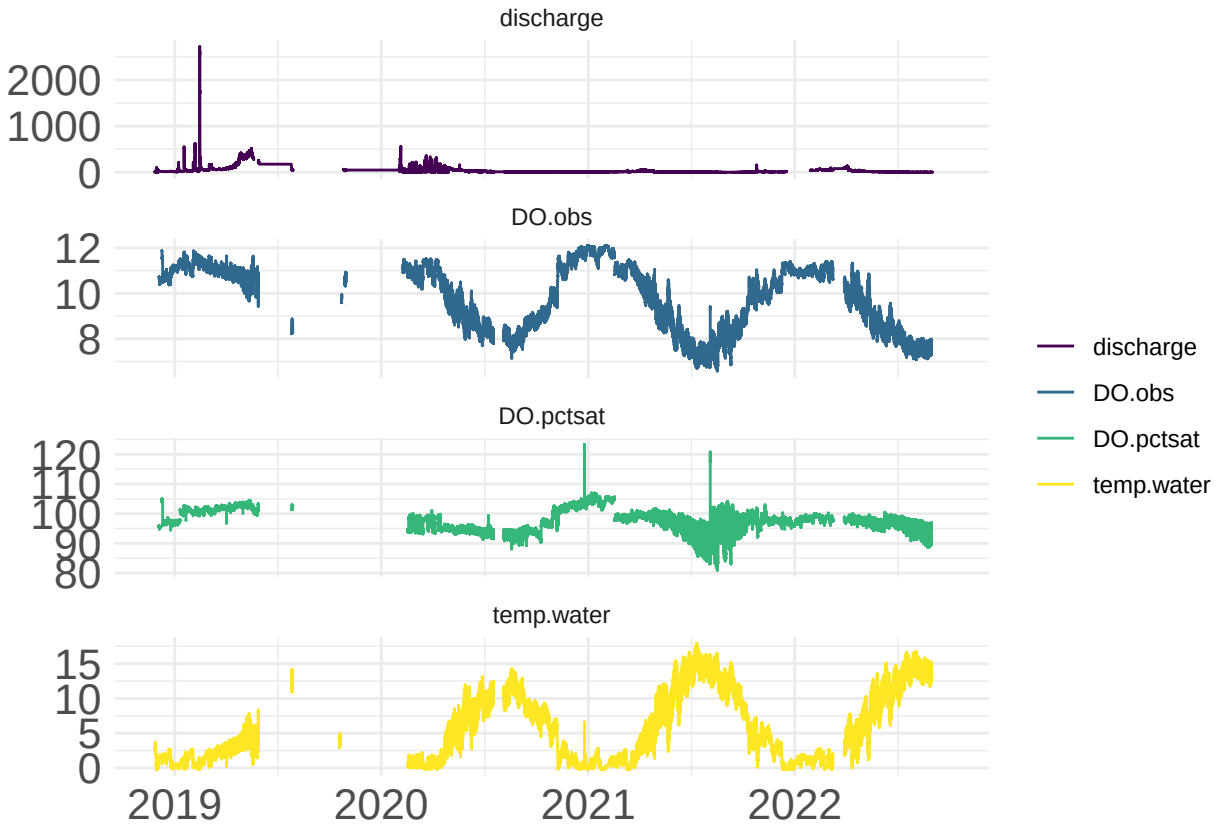


Figure 1: Full metabolism data streams.

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: mm4

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 GPP$\tilde{}$light relationship. Saturating models (e.g., 'mm1sat') assume a saturating GPP$\tilde{}$light relationship. Lastly, Q10 models (e.g., 'mm1satq10') assume a saturating function of GPP$\tilde{}$light and an exponential function of GPP$\tilde{}$Temp. '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	2.700000e+00	370	302	179471.446	-0.707	6546.354
mm1_sat	raw	7.350000e+00	102	138	59767.045	-0.171	2703.517
mm1_satq10	raw	2.640000e+00	82	109	34523.947	-0.512	3269.298
mm2	loess	2.440000e+00	462	219	430.487	0.063	16.772
mm2_sat	loess	2.920000e+00	169	130	430.487	0.151	62.973
mm2_satq10	loess	2.640000e+00	83	100	34523.947	-0.409	700.311
mm3	lm	2.390000e+00	460	222	163.889	0.493	-3.917
mm3_sat	lm	2.570000e+00	208	148	163.889	0.554	26.409
mm3_satq10	lm	2.580000e+00	82	99	34523.947	-0.409	694.098
mm4	mean	2.420000e+00	310	219	38.575	NA	42.139
mm4_sat	mean	3.450000e+00	187	190	1.000	NA	-90.456
mm4_satq10	mean	2.730000e+00	87	99	34523.947	-0.409	738.915
mm5	night	3.037034e+92	605	445	81.613	NA	-2.672
mm5_sat	night	3.873695e+26	199	182	81.790	NA	-22.823
mm5_satq10	night	1.240051e+24	203	171	70.017	NA	-24.759
mm6	empirical-gam	2.714000e+01	108	215	367605.760	-0.286	574493.340
mm6_sat	empirical-gam	2.845000e+01	91	200	367605.760	-0.281	37271.519
mm6_satq10	empirical-gam	6.816000e+01	193	205	367605.760	-0.275	29005.039

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

The most distant from best is: mm1_sat

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:

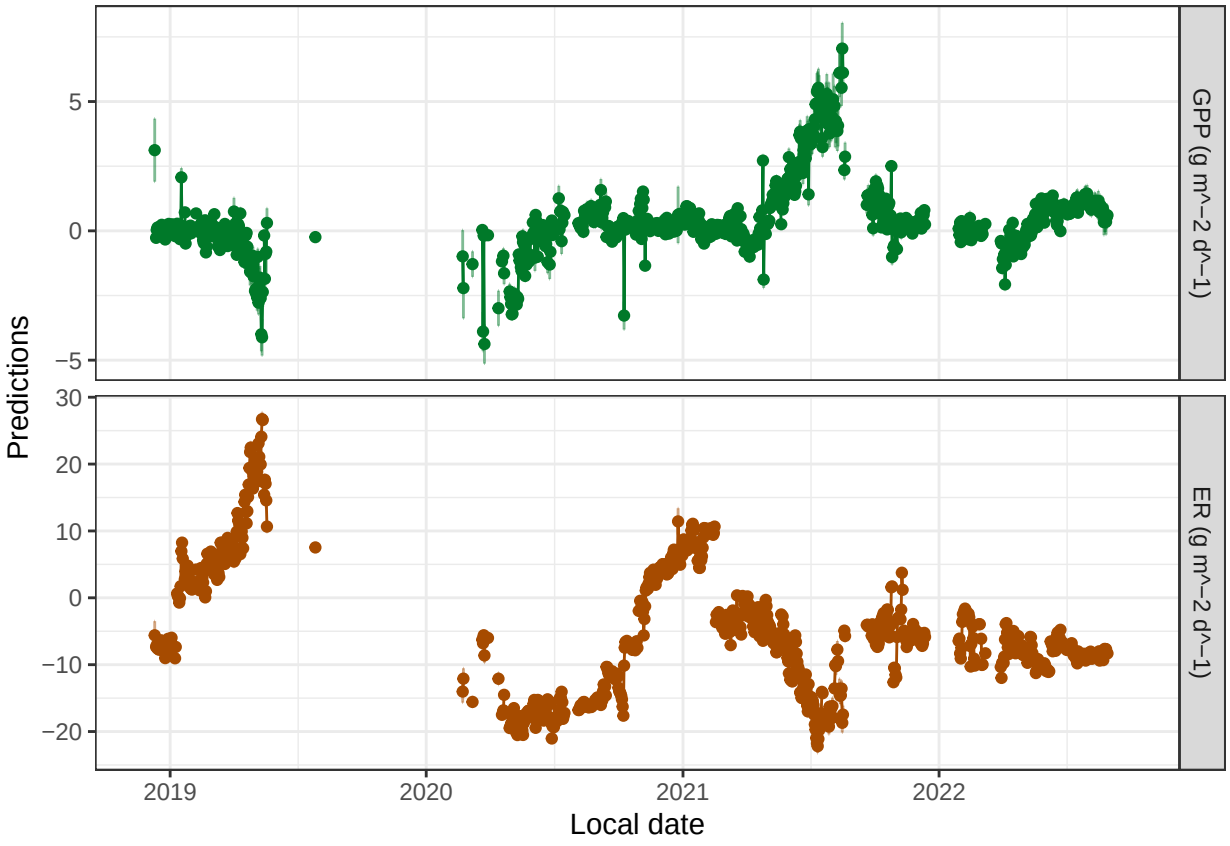


Figure 2: 'Best' model fit.

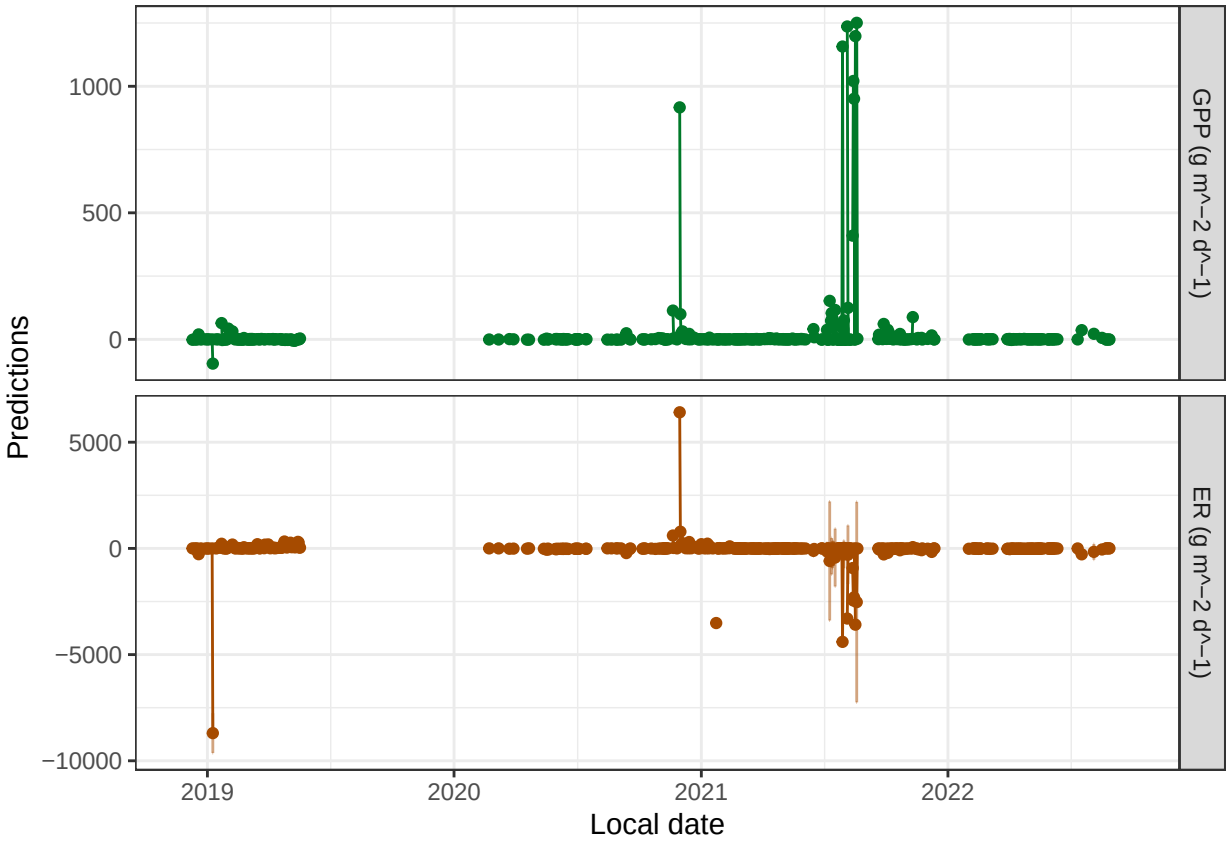


Figure 3: Most distant model.

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 GPP$\tilde{}$light relationship. Saturating models (e.g., 'mm1sat') assume a saturating GPPlight relationship. Lastly, Q10 models (e.g., 'mm1satq10') assume a saturating function of GPP$\tilde{}$light 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_sat	raw	7.35	102	138	59767.045	-0.171	2703.517
mm1_satq10	raw	2.64	82	109	34523.947	-0.512	3269.298
mm2	loess	2.44	462	219	430.487	0.063	16.772
mm2_sat	loess	2.92	169	130	430.487	0.151	62.973
mm2_satq10	loess	2.64	83	100	34523.947	-0.409	700.311
mm3_sat	lm	2.57	208	148	163.889	0.554	26.409
mm3_satq10	lm	2.58	82	99	34523.947	-0.409	694.098
mm4	mean	2.42	310	219	38.575	NA	42.139
mm4_satq10	mean	2.73	87	99	34523.947	-0.409	738.915

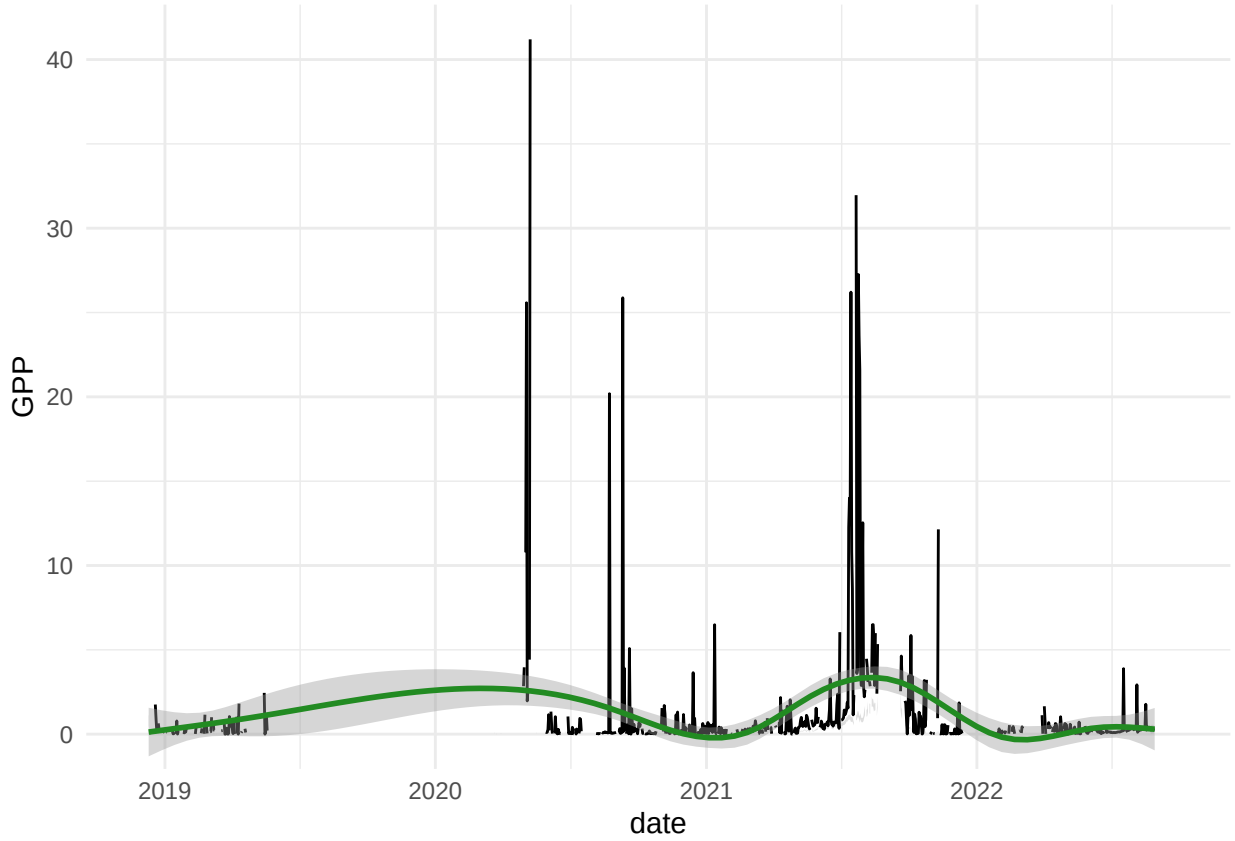
[a] GPPmean = g C m-2 y-1

lowGPP	lowGPPperc	highGPP	highGPPperc	NAs
508	30.059	0	0	600

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

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_sat	raw	7.35	102	138	59767.045	-0.171	2703.517	-4.93	0.012
mm1_satq10	raw	2.64	82	109	34523.947	-0.512	3269.298	-0.22	0.122
mm2	loess	2.44	462	219	430.487	0.063	16.772	-0.02	0.135
mm2_sat	loess	2.92	169	130	430.487	0.151	62.973	-0.50	0.106
mm2_satq10	loess	2.64	83	100	34523.947	-0.409	700.311	-0.22	0.122
mm3_sat	lm	2.57	208	148	163.889	0.554	26.409	-0.15	0.126
mm3_satq10	lm	2.58	82	99	34523.947	-0.409	694.098	-0.16	0.126
mm4	mean	2.42	310	219	38.575	NA	42.139	0.00	0.136
mm4_satq10	mean	2.73	87	99	34523.947	-0.409	738.915	-0.31	0.116


40
30
20
10
0
GPP
2019
2020
2021
2022
date