GUIL GPP model report

2023-01-30

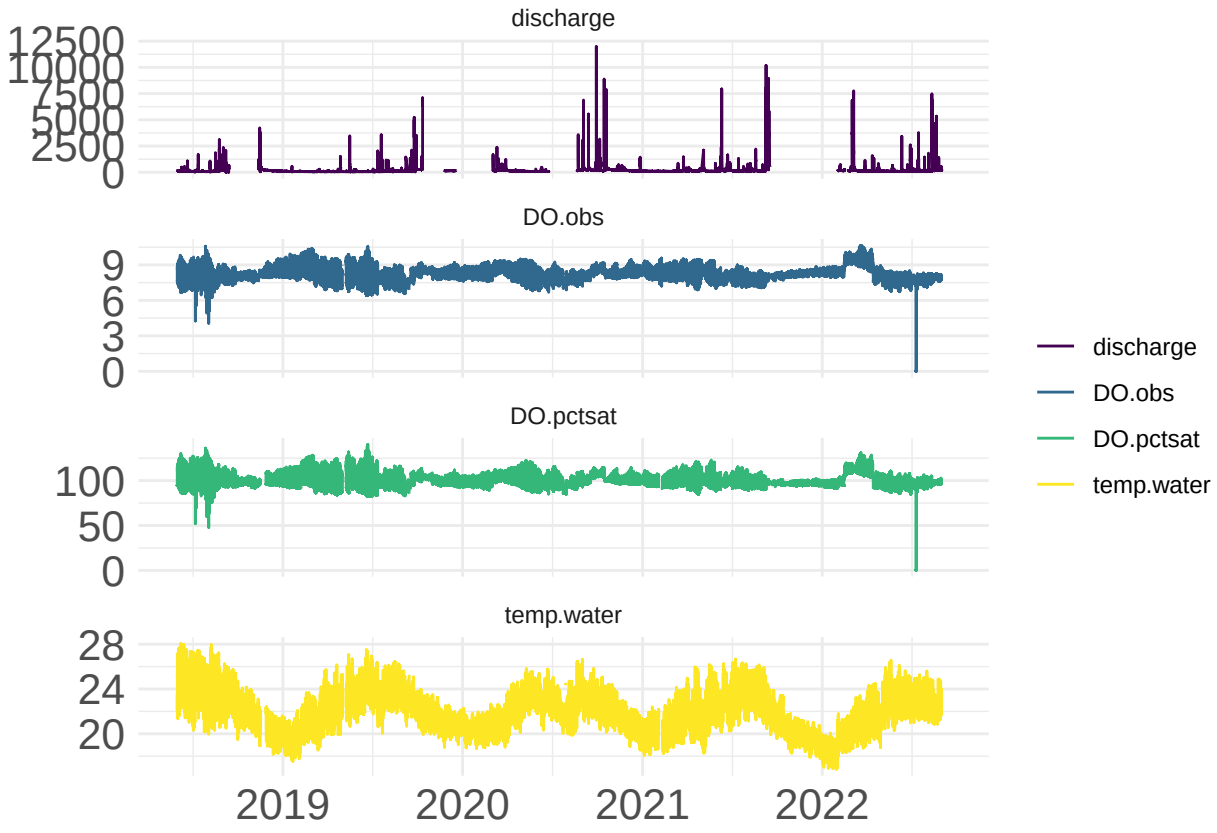


Figure 1: Full metabolism data streams.

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: mm2_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 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	9.650000e+00	29	110	133035.611	-0.974	122742.630
mm1_sat	raw	1.183000e+01	4	49	7057.548	-0.766	35839.132
mm1_satq10	raw	9.140000e+00	3	46	5939.032	-0.728	26032.090
mm2	loess	9.960000e+00	16	108	45.949	-0.182	2775.048
mm2_sat	loess	1.219000e+01	6	59	41.590	-0.186	2334.838
mm2_satq10	loess	8.340000e+00	3	42	1498.259	-0.170	2733.207
mm3	lm	9.980000e+00	8	107	40.094	0.445	2689.380
mm3_sat	lm	1.228000e+01	5	64	29.710	0.390	2242.815
mm3_satq10	lm	8.390000e+00	4	45	1498.259	-0.170	2635.822
mm4	mean	9.980000e+00	8	107	35.584	NA	2684.493
mm4_sat	mean	1.229000e+01	5	65	29.557	NA	2241.016
mm4_satq10	mean	8.380000e+00	3	43	1498.259	-0.170	2619.152
mm5	night	1.332191e+12	201	269	24.054	NA	1429.534
mm5_sat	night	1.523953e+11	46	88	64.339	-0.679	1514.127
mm5_satq10	night	1.934795e+12	43	91	64.339	-0.557	1489.541
mm6	empirical-gam	1.605000e+02	88	145	520655.974	-0.065	2766232.659
mm6_sat	empirical-gam	1.451600e+02	138	142	520655.974	-0.265	13421.651
mm6_satq10	empirical-gam	1.443200e+02	140	144	520655.974	-0.266	13986.755

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

The most distant from best is: mm4_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:

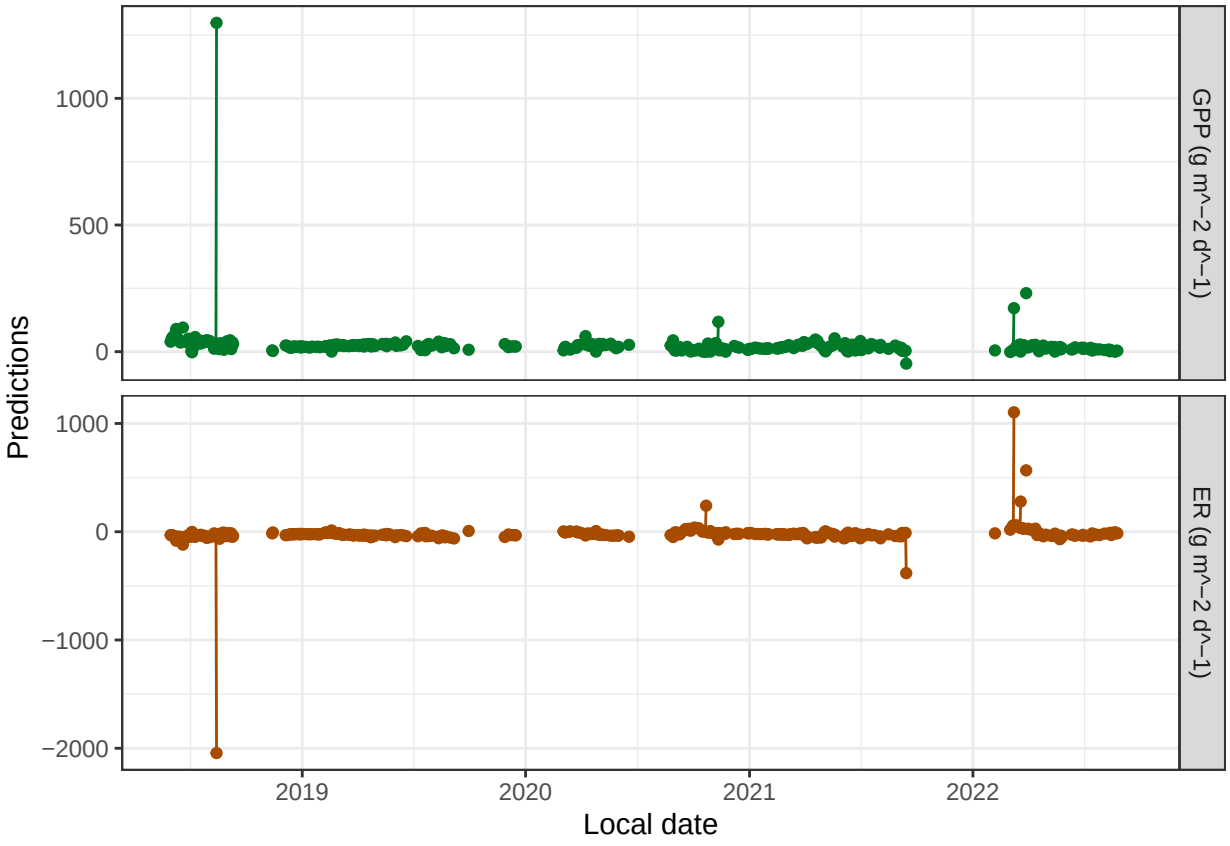


Figure 2: 'Best' model fit.

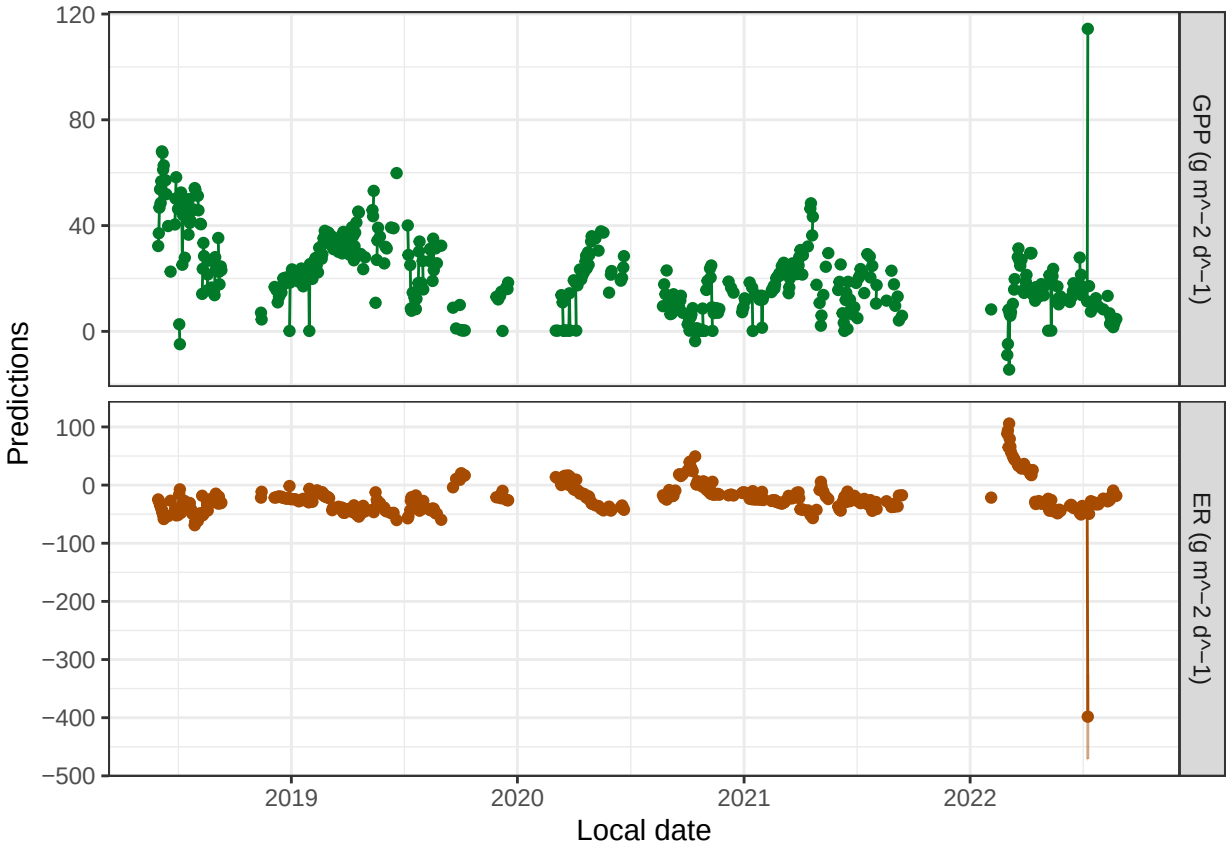


Figure 3: Most distant model.

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
mm2	loess	9.96	16	108	45.949	-0.182	2775.048
mm2_sat	loess	12.19	6	59	41.590	-0.186	2334.838
mm2_satq10	loess	8.34	3	42	1498.259	-0.170	2733.207
mm3	lm	9.98	8	107	40.094	0.445	2689.380
mm3_sat	lm	12.28	5	64	29.710	0.390	2242.815
mm3_satq10	lm	8.39	4	45	1498.259	-0.170	2635.822
mm4	mean	9.98	8	107	35.584	NA	2684.493
mm4_sat	mean	12.29	5	65	29.557	NA	2241.016
mm4_satq10	mean	8.38	3	43	1498.259	-0.170	2619.152

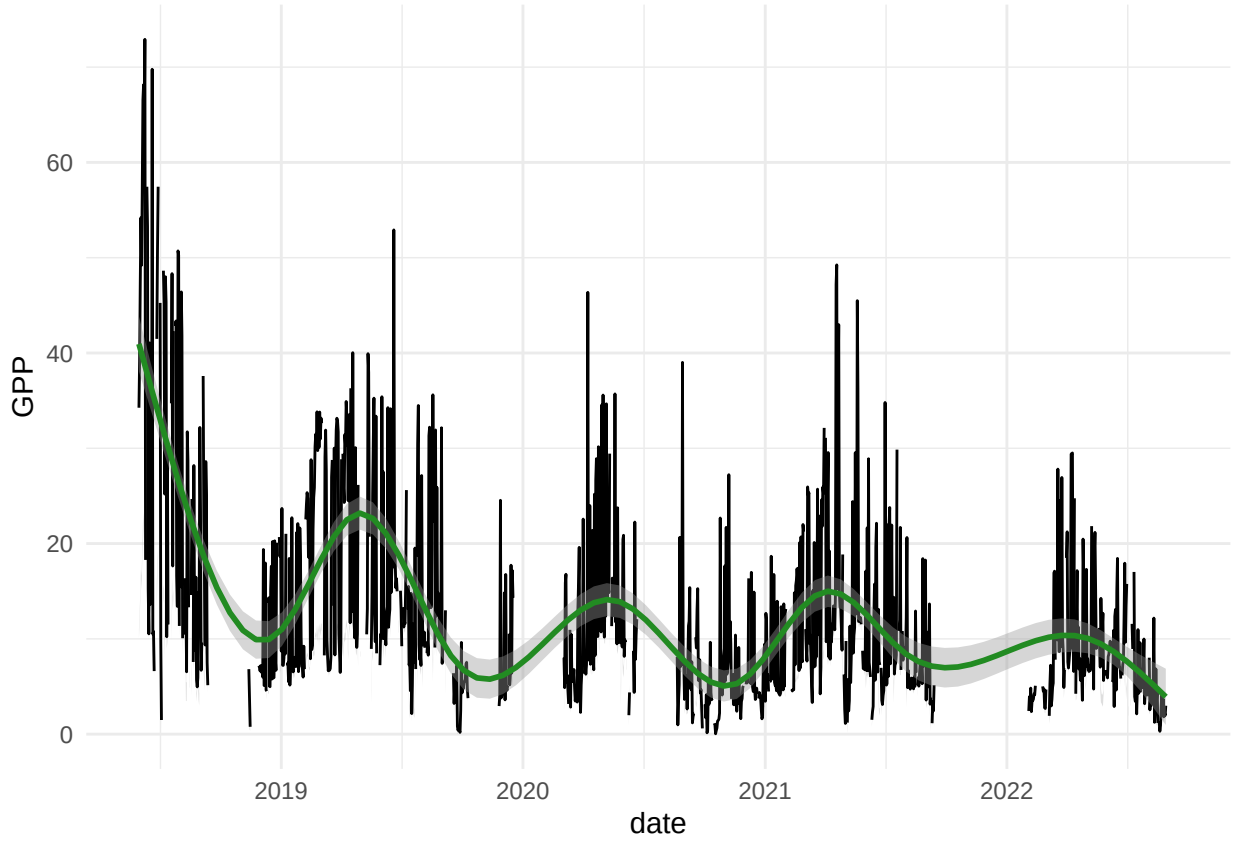
[a] GPPmean = g C m-2 y-1

lowGPP	lowGPPperc	highGPP	highGPPperc	NAs
6	0.779	72	9.351	2364

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

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

modelID	modelType	RMSE	negativeGPP	positiveER	maxK	ER.Kcorr	meanGPP	dRMSE	RMSEwt
mm2	loess	9.96	16	108	45.949	-0.182	2775.048	-1.62	0.095
mm2_sat	loess	12.19	6	59	41.590	-0.186	2334.838	-3.85	0.031
mm2_satq10	loess	8.34	3	42	1498.259	-0.170	2733.207	0.00	0.213
mm3	lm	9.98	8	107	40.094	0.445	2689.380	-1.64	0.094
mm3_sat	lm	12.28	5	64	29.710	0.390	2242.815	-3.94	0.030
mm3_satq10	lm	8.39	4	45	1498.259	-0.170	2635.822	-0.05	0.207
mm4	mean	9.98	8	107	35.584	NA	2684.493	-1.64	0.094
mm4_sat	mean	12.29	5	65	29.557	NA	2241.016	-3.95	0.029
mm4_satq10	mean	8.38	3	43	1498.259	-0.170	2619.152	-0.04	0.208


GPP
60
40
20
0
2019
2020
2021
2022
date