PRIN GPP model report

2023-02-01

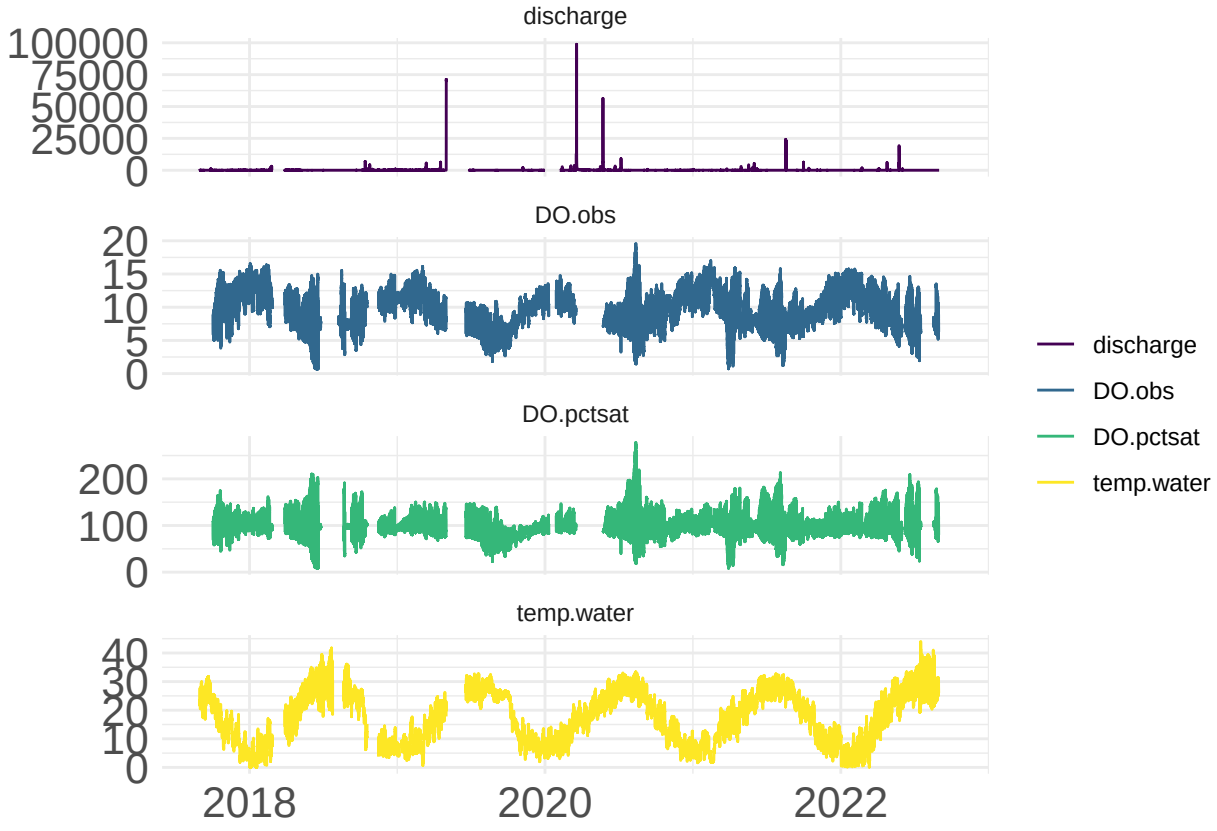


Figure 1: Full metabolism data streams.

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: mm1

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	2.452000e+01	21	17	28907.703	-0.940	2487.217
mm1_sat	raw	2.486000e+01	17	15	2412.766	-0.590	1600.604
mm1_satq10	raw	2.570000e+01	17	15	167692.782	-0.996	1417.894
mm2	loess	2.704000e+01	44	26	10.797	-0.129	1004.163
mm2_sat	loess	2.945000e+01	27	75	10.720	-0.038	822.510
mm2_satq10	loess	2.866000e+01	26	75	2755.616	-0.449	902.837
mm3	lm	2.731000e+01	53	27	7.315	0.269	1006.657
mm3_sat	lm	2.887000e+01	29	56	10.442	0.212	852.864
mm3_satq10	lm	2.825000e+01	30	62	2755.616	-0.449	909.090
mm4	mean	2.730000e+01	53	27	6.955	NA	1007.115
mm4_sat	mean	2.957000e+01	34	68	6.690	NA	844.332
mm4_satq10	mean	2.845000e+01	32	73	2755.616	-0.449	907.331
mm5	night	2.317054e+20	37	64	9.007	-1.000	1140.298
mm5_sat	night	3.216000e+01	21	96	1184.896	NA	949.061
mm5_satq10	night	1.527885e+05	20	93	982.867	NA	928.407
mm6	empirical-gam	4.206300e+02	157	43	127481.288	-0.266	3325838.427
mm6_sat	empirical-gam	4.179100e+02	157	74	127481.288	-0.314	24073.887
mm6_satq10	empirical-gam	4.218900e+02	185	80	127481.288	-0.320	21719.388

[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:

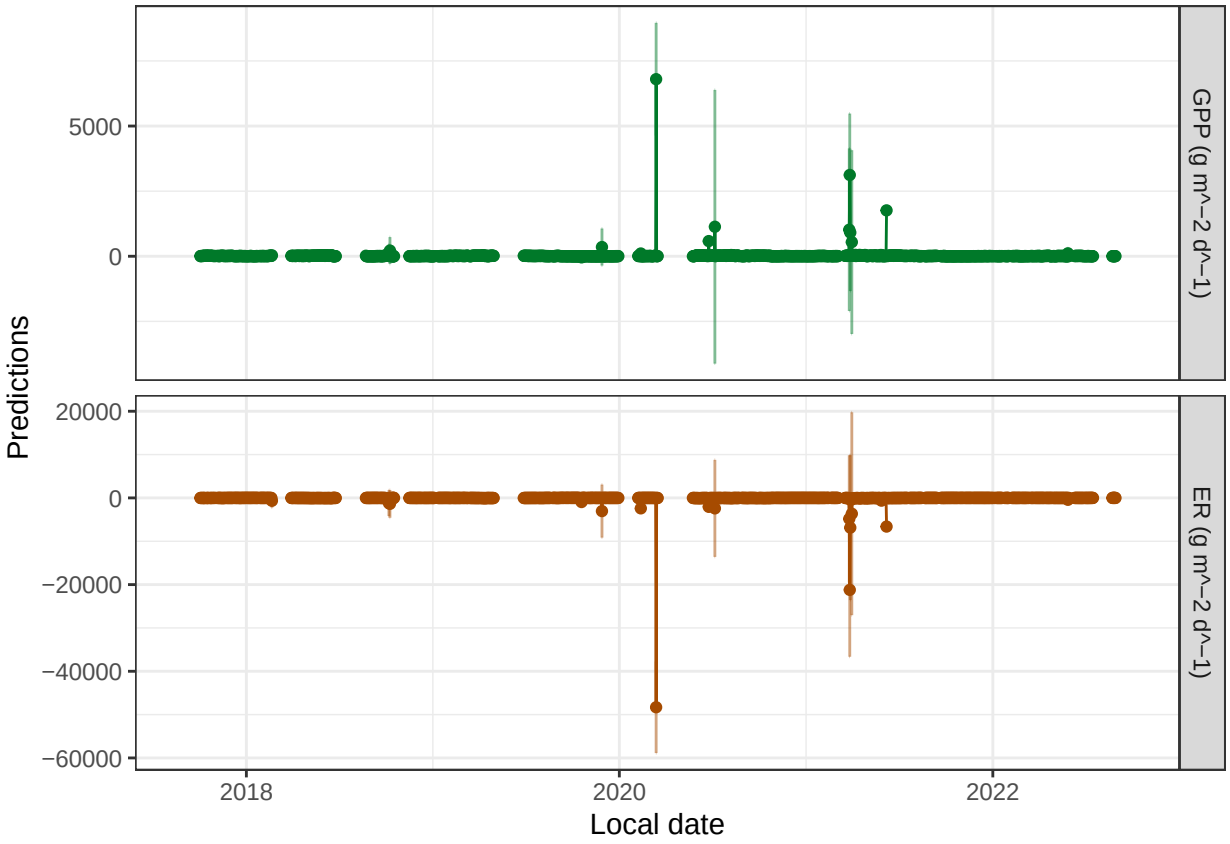


Figure 2: 'Best' model fit.

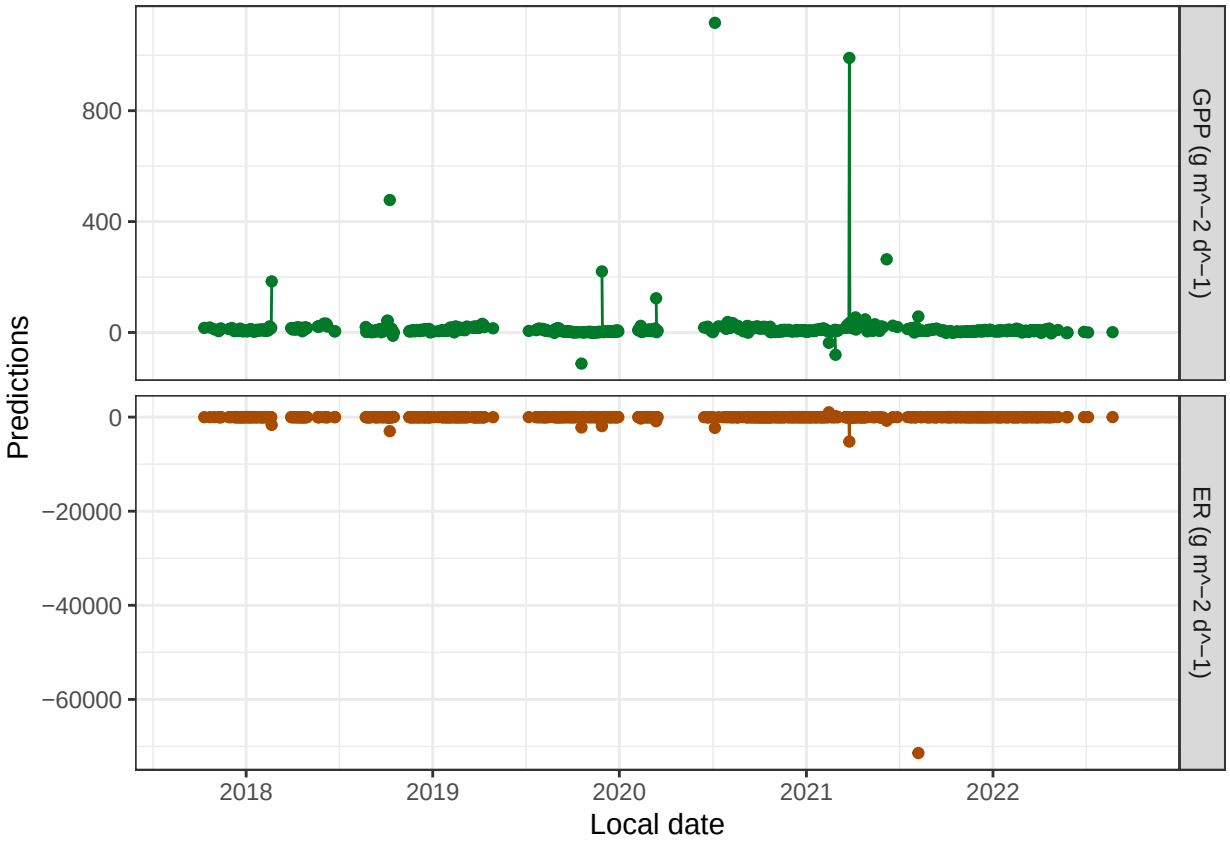


Figure 3: Most distant model.

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 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	raw	24.52	21	17	28907.703	-0.940	2487.217
mm1_sat	raw	24.86	17	15	2412.766	-0.590	1600.604
mm1_satq10	raw	25.70	17	15	167692.782	-0.996	1417.894
mm2	loess	27.04	44	26	10.797	-0.129	1004.163
mm2_sat	loess	29.45	27	75	10.720	-0.038	822.510
mm2_satq10	loess	28.66	26	75	2755.616	-0.449	902.837
mm3	lm	27.31	53	27	7.315	0.269	1006.657
mm3_sat	lm	28.87	29	56	10.442	0.212	852.864
mm3_satq10	lm	28.25	30	62	2755.616	-0.449	909.090
mm4	mean	27.30	53	27	6.955	NA	1007.115
mm4_sat	mean	29.57	34	68	6.690	NA	844.332
mm4_satq10	mean	28.45	32	73	2755.616	-0.449	907.331

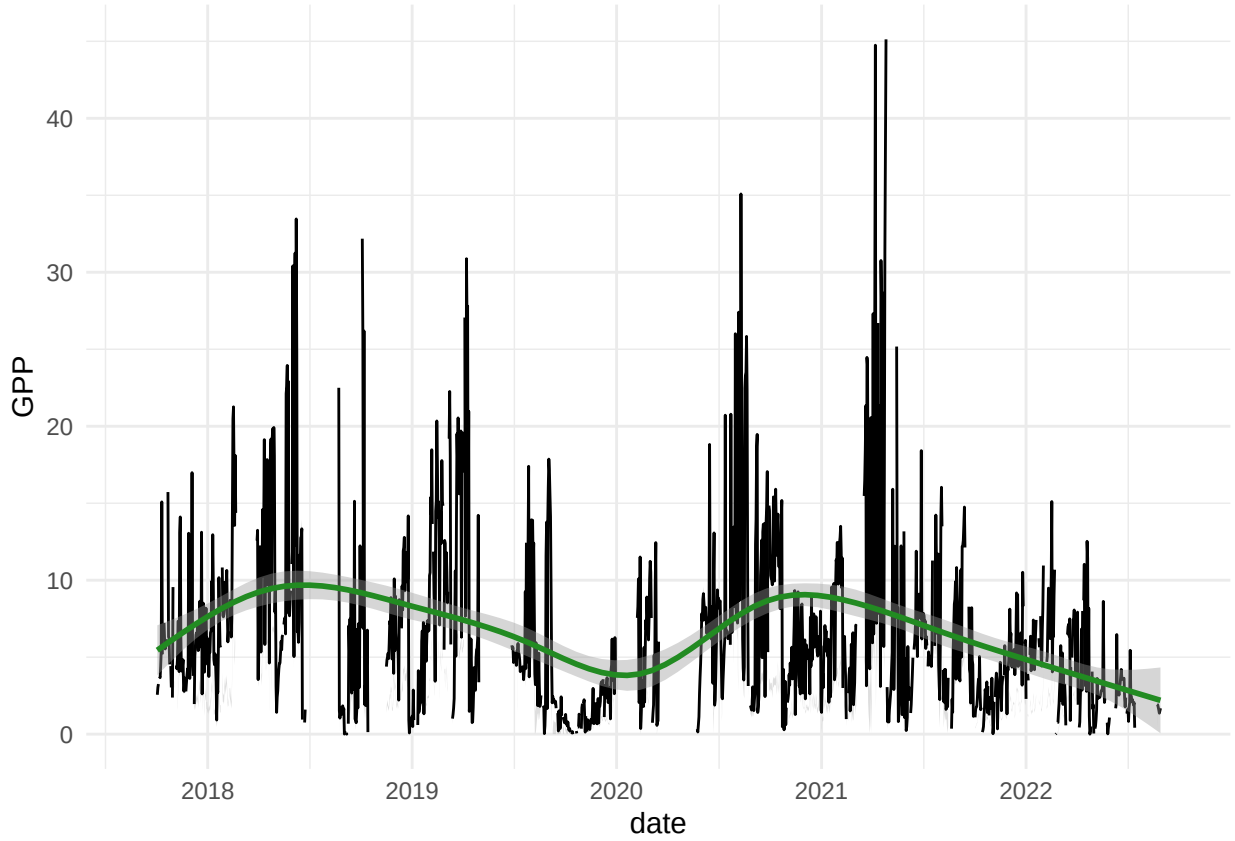
[a] GPPmean = g C m-2 y-1

lowGPP	lowGPPperc	highGPP	highGPPperc	NAs
40	1.496	58	2.169	934

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

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	24.86	17	15	2412.766	-0.590	1600.604	0.00	0.363
mm2	loess	27.04	44	26	10.797	-0.129	1004.163	-2.18	0.122
mm2_sat	loess	29.45	27	75	10.720	-0.038	822.510	-4.59	0.037
mm2_satq10	loess	28.66	26	75	2755.616	-0.449	902.837	-3.80	0.054
mm3	lm	27.31	53	27	7.315	0.269	1006.657	-2.45	0.107
mm3_sat	lm	28.87	29	56	10.442	0.212	852.864	-4.01	0.049
mm3_satq10	lm	28.25	30	62	2755.616	-0.449	909.090	-3.39	0.067
mm4	mean	27.30	53	27	6.955	NA	1007.115	-2.44	0.107
mm4_sat	mean	29.57	34	68	6.690	NA	844.332	-4.71	0.034
mm4_satq10	mean	28.45	32	73	2755.616	-0.449	907.331	-3.59	0.060


40
30
20
10
0
GPP
2018
2019
2020
2021
2022
date