MCDI GPP model report

2023-01-31

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_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	20.94	22	81	1.045285e+04	-0.160	4847.781
mm1_sat	raw	16.78	19	76	3.441419e+04	-0.927	5770.664
mm1_satq10	raw	17.31	19	73	2.684377e+03	-0.751	4554.097
mm2	loess	22.10	19	67	2.831000e+01	-0.329	1510.927
mm2_sat	loess	20.11	19	56	-Inf	1.000	1629.686
mm2_satq10	loess	18.07	21	67	2.684377e+03	-0.996	2173.766
mm3	lm	23.27	28	66	1.493480e+02	-0.402	1213.241
mm3_sat	lm	19.75	20	59	1.633150e+02	-0.403	1345.071
mm3_satq10	lm	18.19	21	69	2.684377e+03	-0.996	1967.386
mm4	mean	25.42	25	67	1.288000e+01	NA	1258.272
mm4_sat	mean	23.22	19	62	1.493400e+01	NA	1350.256
mm4_satq10	mean	18.84	21	68	2.684377e+03	-0.996	2015.286
mm5	night	106911.41	55	147	6.078400e+01	-0.280	1529.552
mm5_sat	night	138.00	25	98	6.078400e+01	-0.195	1565.620
mm5_satq10	night	20.92	25	92	6.078400e+01	-0.230	1545.300
mm6	empirical-lm	917.47	151	82	6.481758e+16	0.048	774677.607
mm6_sat	empirical-lm	778.52	82	96	6.481758e+16	0.070	20541.605
mm6_satq10	empirical-lm	785.85	75	94	6.481758e+16	0.048	20648.361

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

The most distant from best is: mm2_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:

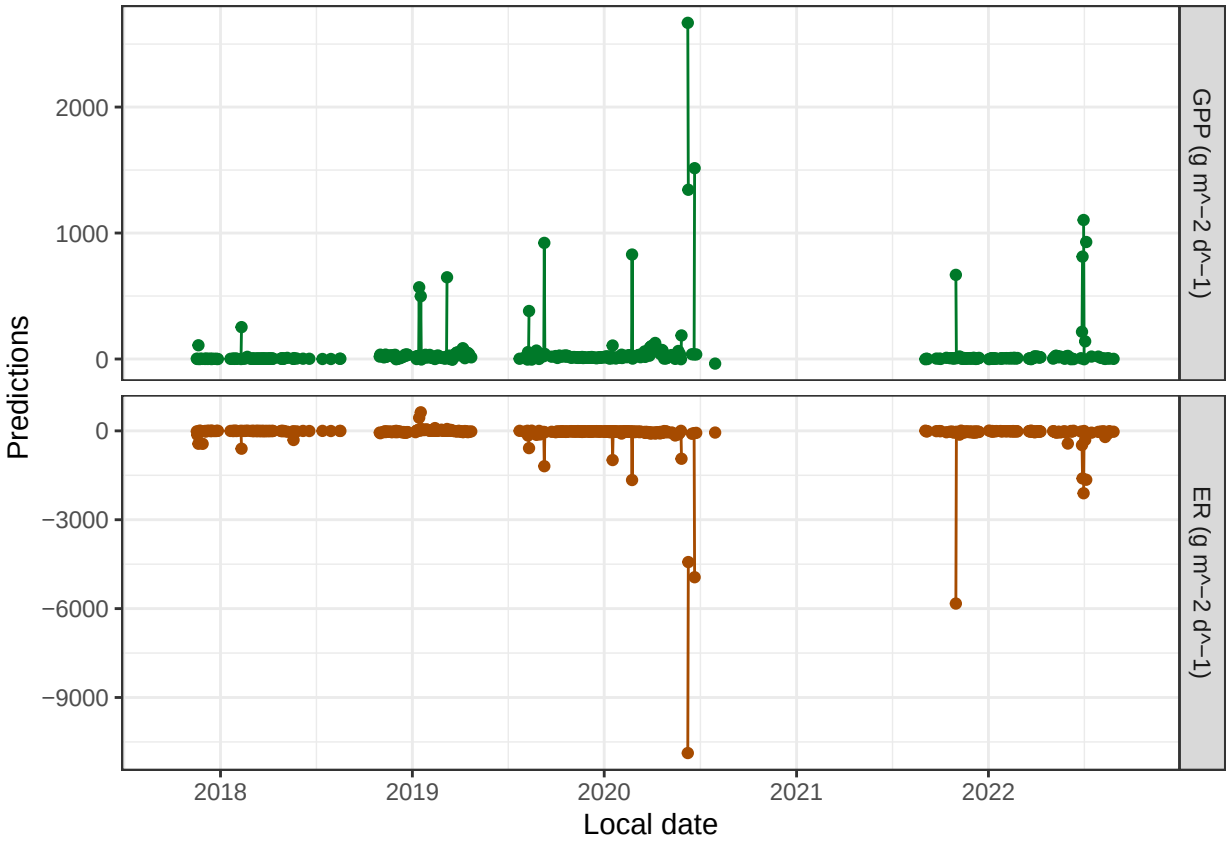

Figure 2: 'Best' model fit.

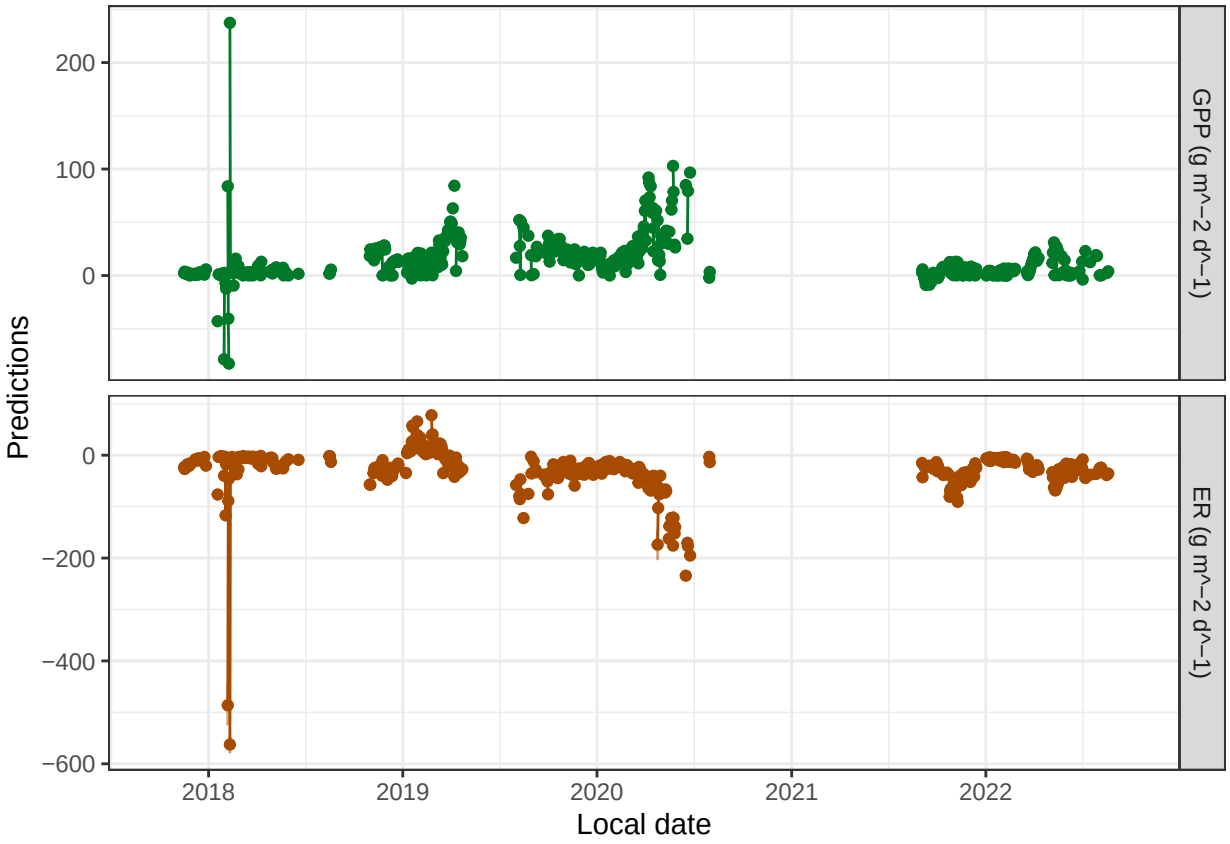

Figure 3: Most distant model.

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	raw	20.94	22	81	10452.849	-0.160	4847.781
mm1_satq10	raw	17.31	19	73	2684.377	-0.751	4554.097
mm2	loess	22.10	19	67	28.310	-0.329	1510.927
mm2_sat	loess	20.11	19	56	-Inf	1.000	1629.686
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mm3	lm	23.27	28	66	149.348	-0.402	1213.241
mm3_sat	lm	19.75	20	59	163.315	-0.403	1345.071
mm3_satq10	lm	18.19	21	69	2684.377	-0.996	1967.386
mm4_sat	mean	23.22	19	62	14.934	NA	1350.256
mm4_satq10	mean	18.84	21	68	2684.377	-0.996	2015.286
mm5_satq10	night	20.92	25	92	60.784	-0.230	1545.300

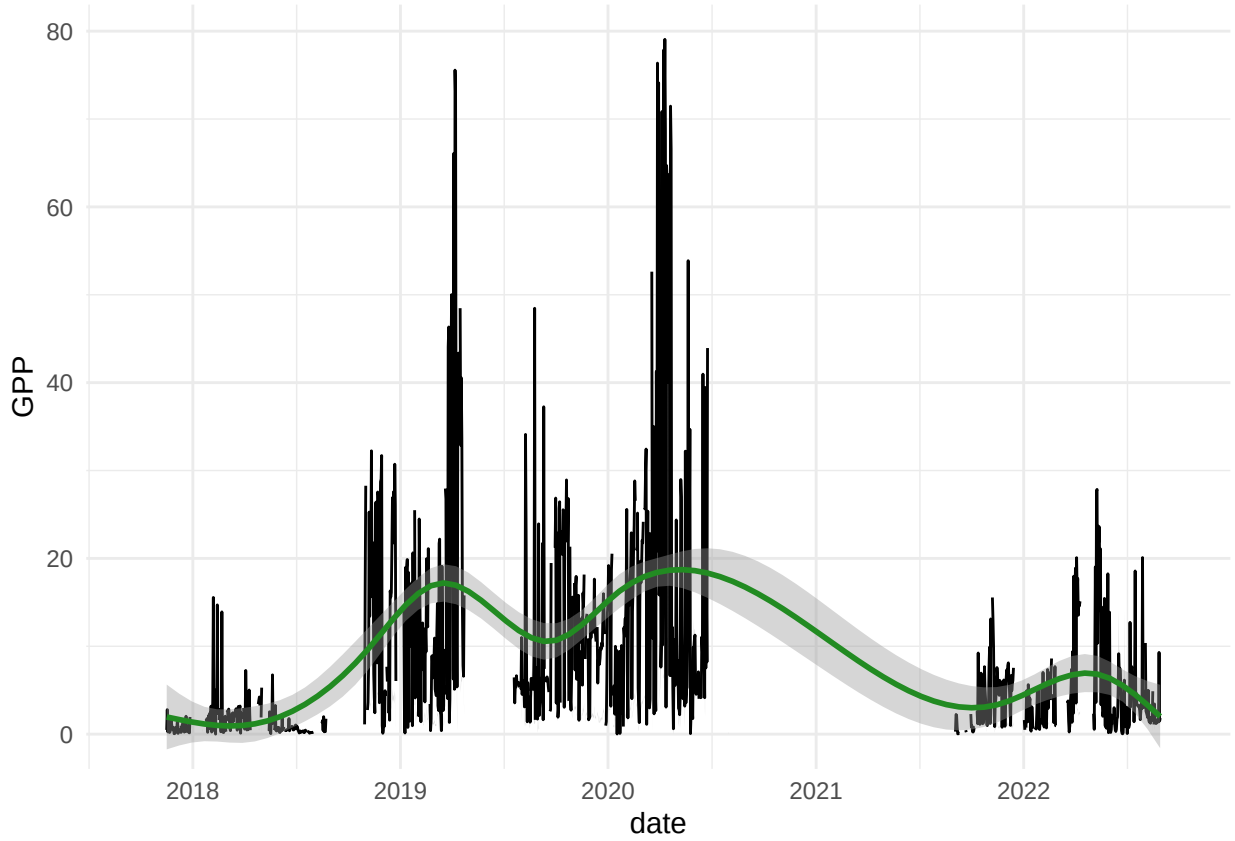
[a] GPPmean = g C m-2 y-1

lowGPP	lowGPPperc	highGPP	highGPPperc	NAs
34	3.295	118	11.434	2582

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

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	raw	20.94	22	81	10452.849	-0.160	4847.781	-3.63	0.090
mm1_satq10	raw	17.31	19	73	2684.377	-0.751	4554.097	0.00	0.550
mm2	loess	22.10	19	67	28.310	-0.329	1510.927	-4.79	0.050
mm3	lm	23.27	28	66	149.348	-0.402	1213.241	-5.96	0.028
mm3_sat	lm	19.75	20	59	163.315	-0.403	1345.071	-2.44	0.163
mm4_sat	mean	23.22	19	62	14.934	NA	1350.256	-5.91	0.029
mm5_satq10	night	20.92	25	92	60.784	-0.230	1545.300	-3.61	0.091


80
60
40
20
0
GPP
2018
2019
2020
2021
2022
date