WALK GPP model report

2023-02-01

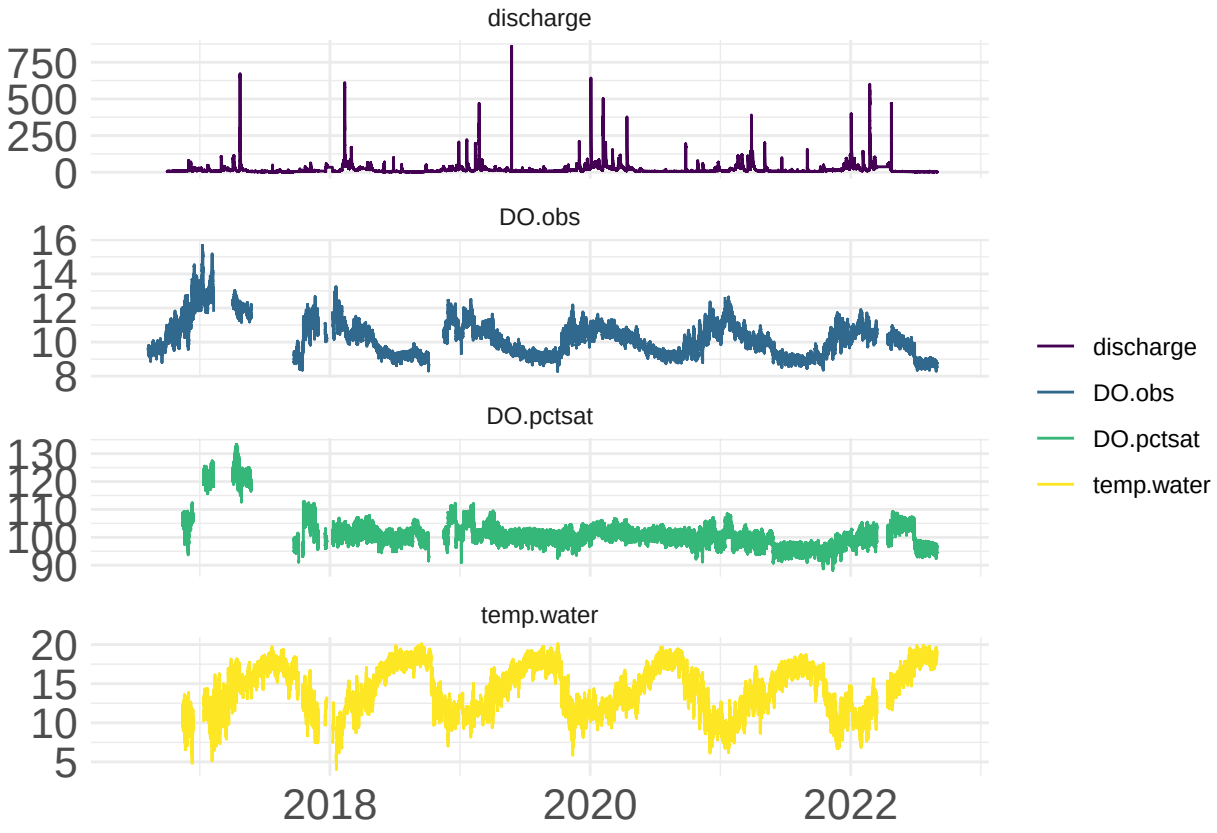


Figure 1: Full metabolism data streams.

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: mm2

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	3.070000e+00	322	586	201511.242	-0.234	15394.687
mm1_sat	raw	3.220000e+00	103	292	31487.937	-0.459	7625.721
mm1_satq10	raw	3.410000e+00	86	271	137024.151	0.762	7942.006
mm2	loess	3.010000e+00	61	493	-Inf	NA	171.875
mm2_sat	loess	3.130000e+00	30	292	51.048	0.030	203.946
mm2_satq10	loess	3.270000e+00	88	264	137024.151	0.998	634.467
mm3	lm	3.020000e+00	53	486	29.633	0.150	138.636
mm3_sat	lm	3.110000e+00	30	322	39.611	-0.065	194.662
mm3_satq10	lm	3.200000e+00	87	267	137024.151	0.998	592.305
mm4	mean	3.020000e+00	56	486	24.728	NA	138.564
mm4_sat	mean	3.120000e+00	26	305	30.320	NA	197.439
mm4_satq10	mean	3.220000e+00	85	264	137024.151	0.998	584.227
mm5	night	1.518053e+14	589	710	-Inf	NA	112.353
mm5_sat	night	2.626729e+09	217	325	91.159	0.029	76.909
mm5_satq10	night	3.503858e+07	212	323	91.159	0.003	73.759
mm6	empirical-gam	4.374000e+01	76	542	180367.501	-0.161	747442.642
mm6_sat	empirical-gam	3.738000e+01	38	564	180367.501	-0.079	44700.369
mm6_satq10	empirical-gam	6.516000e+01	62	576	180367.501	-0.121	46612.028

[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:

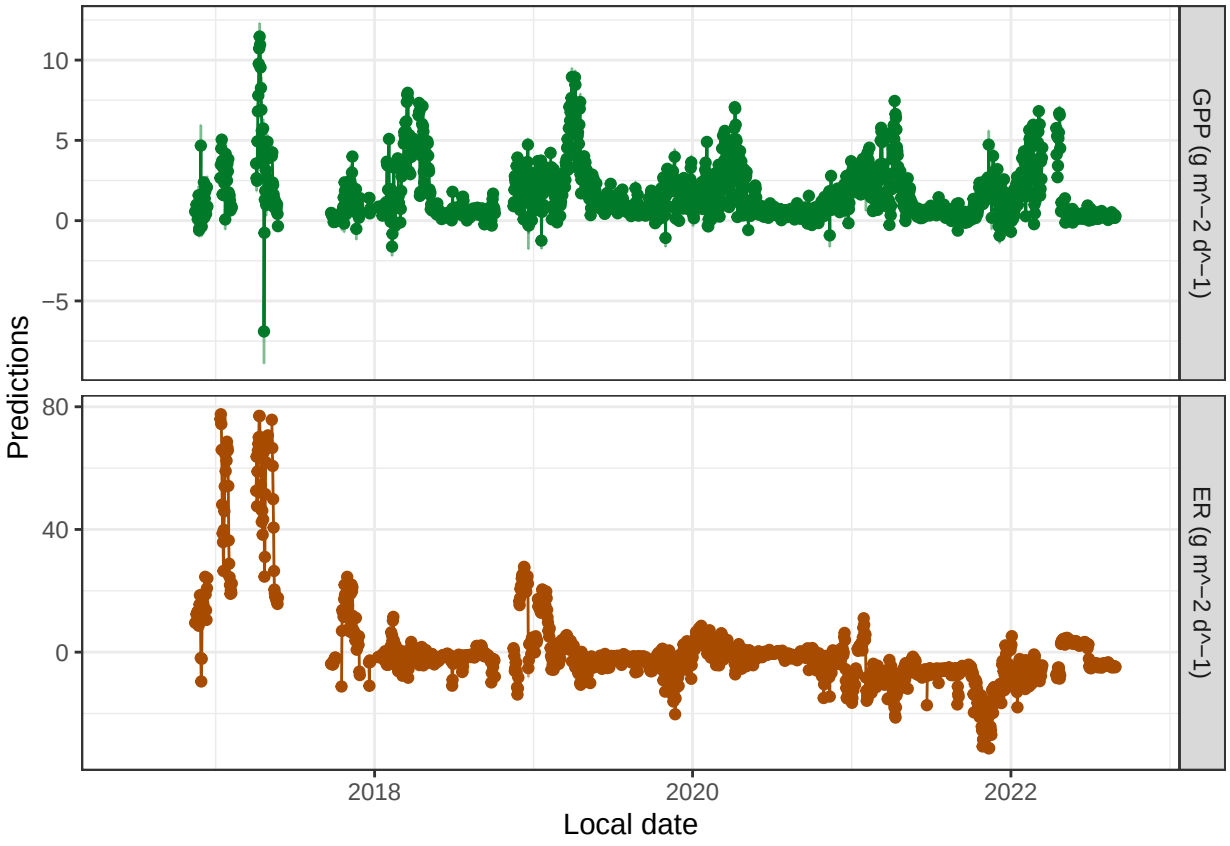


Figure 2: 'Best' model fit.

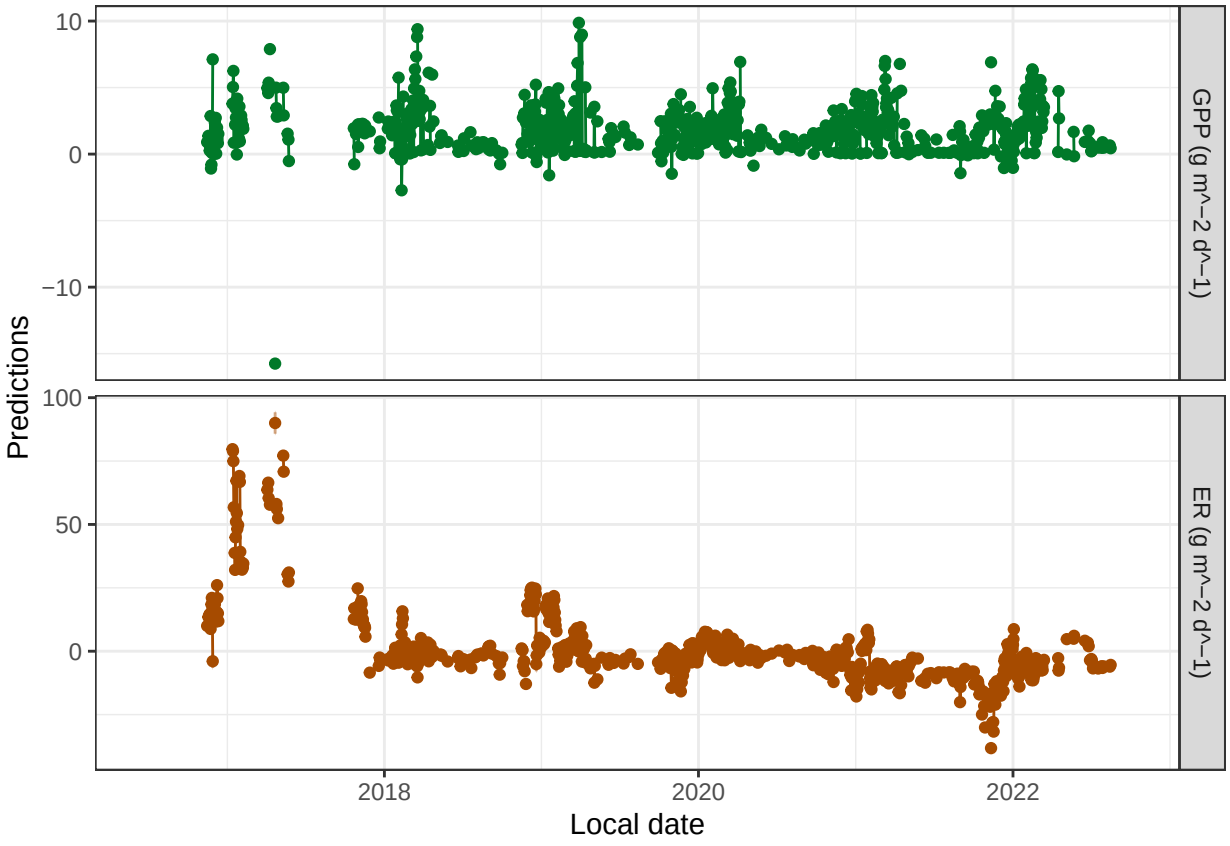


Figure 3: Most distant model.

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
mm2	loess	3.01	61	493	-Inf	NA	171.875
mm2_sat	loess	3.13	30	292	51.048	0.030	203.946
mm2_satq10	loess	3.27	88	264	137024.151	0.998	634.467
mm3	lm	3.02	53	486	29.633	0.150	138.636
mm3_sat	lm	3.11	30	322	39.611	-0.065	194.662
mm3_satq10	lm	3.20	87	267	137024.151	0.998	592.305
mm4	mean	3.02	56	486	24.728	NA	138.564
mm4_sat	mean	3.12	26	305	30.320	NA	197.439
mm4_satq10	mean	3.22	85	264	137024.151	0.998	584.227

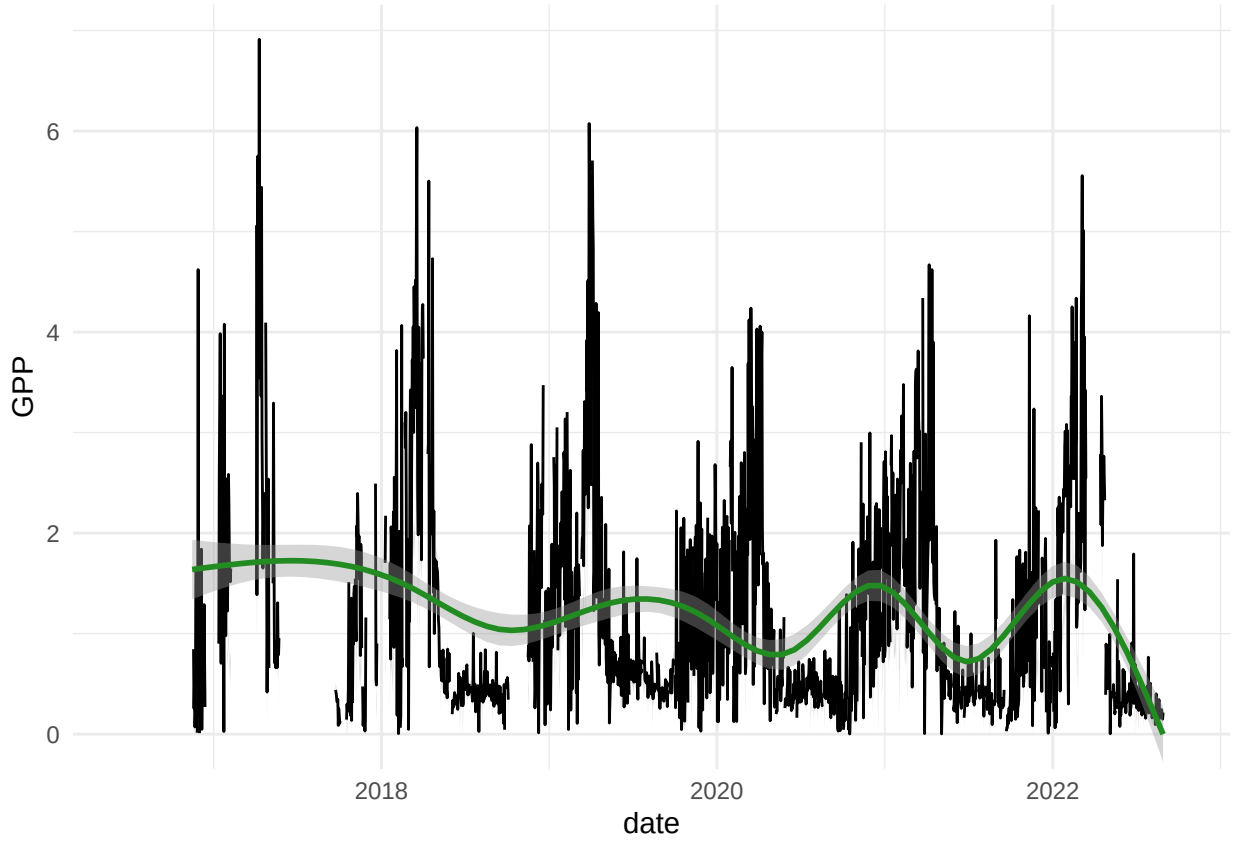
[a] GPPmean = g C m-2 y-1

lowGPP	lowGPPperc	highGPP	highGPPperc	NAs
80	2.358	0	0	1052

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

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	3.01	61	493	-Inf	NA	171.875	0.00	0.172
mm2_sat	loess	3.13	30	292	51.048	0.030	203.946	-0.12	0.162
mm3	lm	3.02	53	486	29.633	0.150	138.636	-0.01	0.171
mm3_sat	lm	3.11	30	322	39.611	-0.065	194.662	-0.10	0.163
mm4	mean	3.02	56	486	24.728	NA	138.564	-0.01	0.171
mm4_sat	mean	3.12	26	305	30.320	NA	197.439	-0.11	0.162


GPP
6
4
2
0
2018
2020
2022
date