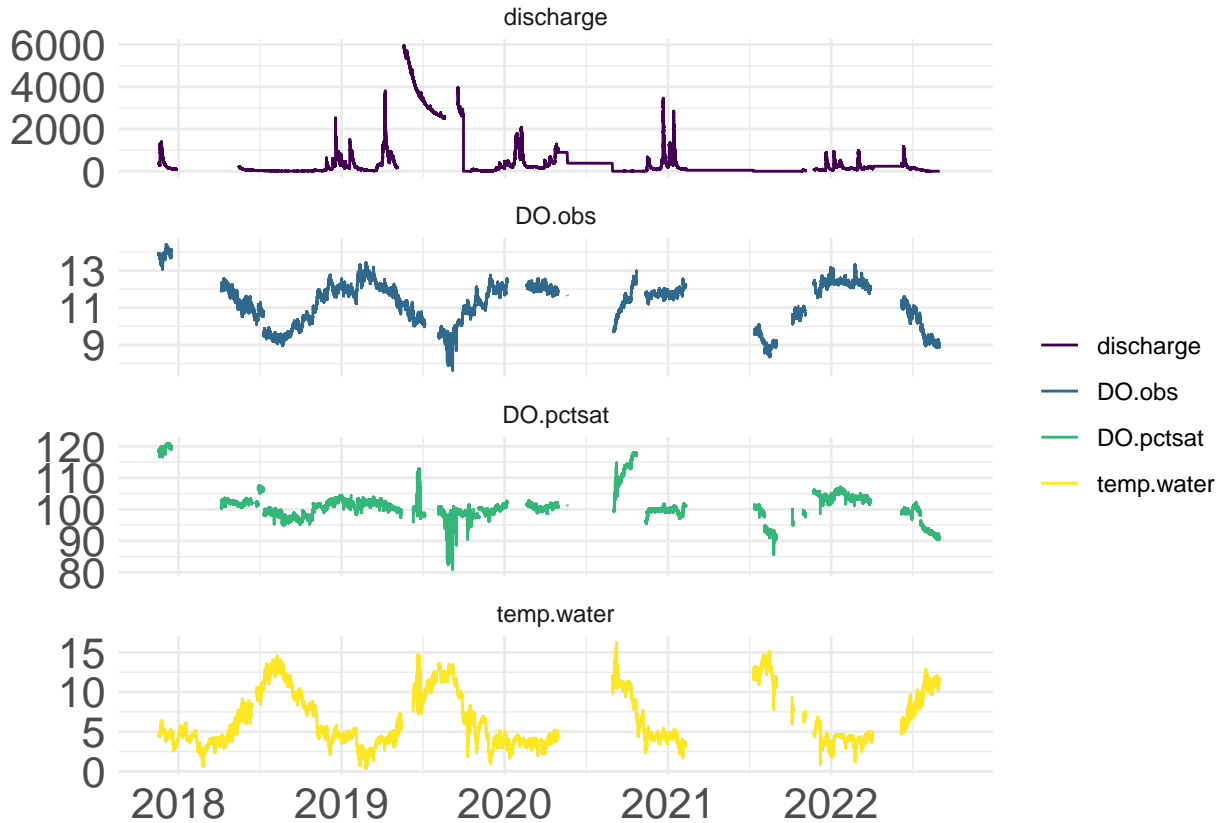# MCRA GPP model report

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

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	1.180000e+00	467	504	143720.807	-0.904	540.604
mm1_sat	raw	1.650000e+00	170	271	85968.017	-0.603	92.180
mm1_satq10	raw	1.670000e+00	180	281	245690.171	-0.260	745.243
mm2	loess	1.250000e+00	617	510	26.991	0.234	-32.163
mm2_sat	loess	1.330000e+00	272	277	26.991	0.240	-16.236
mm2_satq10	loess	1.310000e+00	286	276	26.991	0.225	-17.019
mm3	lm	1.290000e+00	607	508	22.923	0.208	-23.678
mm3_sat	lm	1.400000e+00	271	271	22.923	0.262	-11.317
mm3_satq10	lm	1.350000e+00	288	270	22.923	0.271	-17.360
mm4	mean	1.290000e+00	599	509	18.506	NA	-26.223
mm4_sat	mean	1.440000e+00	199	215	1.000	NA	-35.752
mm4_satq10	mean	1.460000e+00	215	205	245690.171	-0.090	-367.793
mm5	night	2.502500e+41	574	439	0.936	NA	58.684
mm5_sat	night	4.261891e+42	227	181	79.536	0.457	-27.994
mm5_satq10	night	9.784297e+37	247	183	79.536	0.414	-32.616

ᵃ GPPmean = g C m-2 y-1

The most distant from best is: mm5

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:
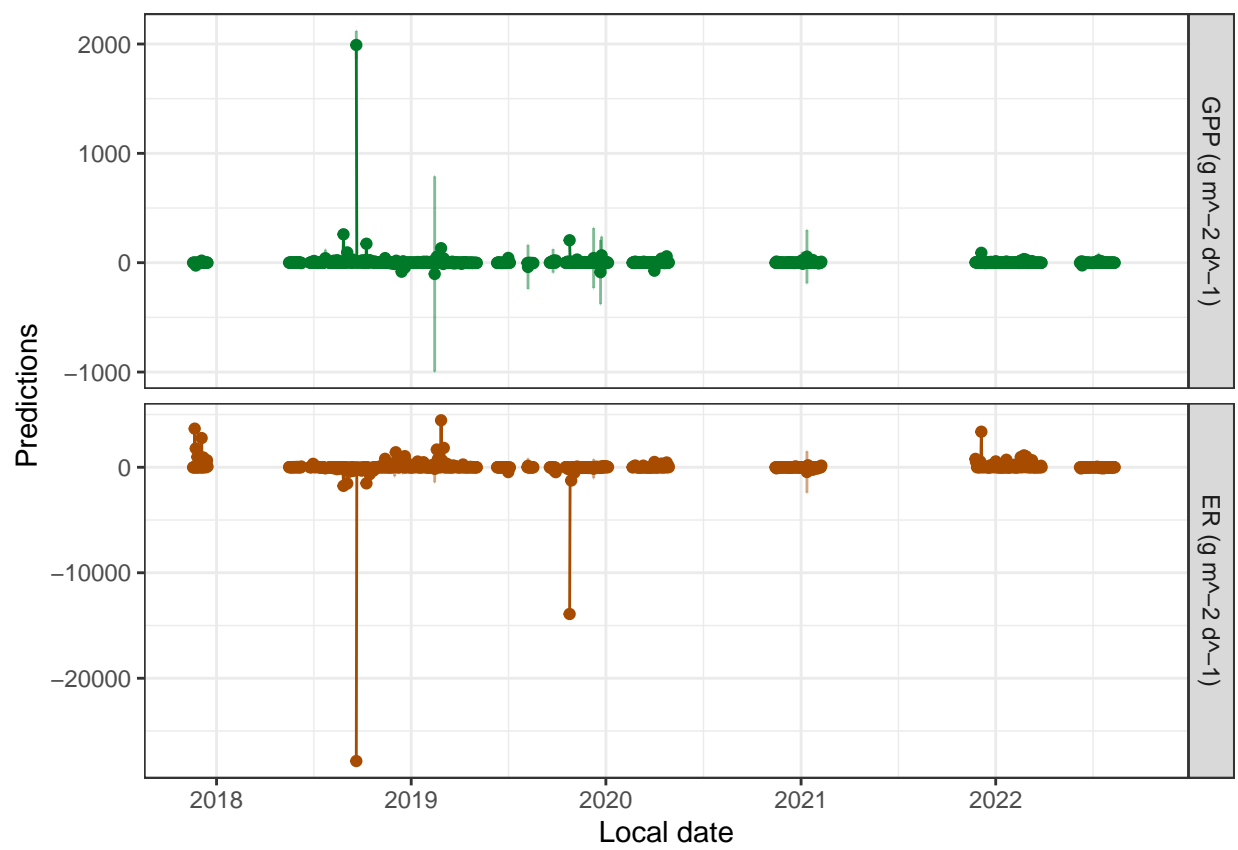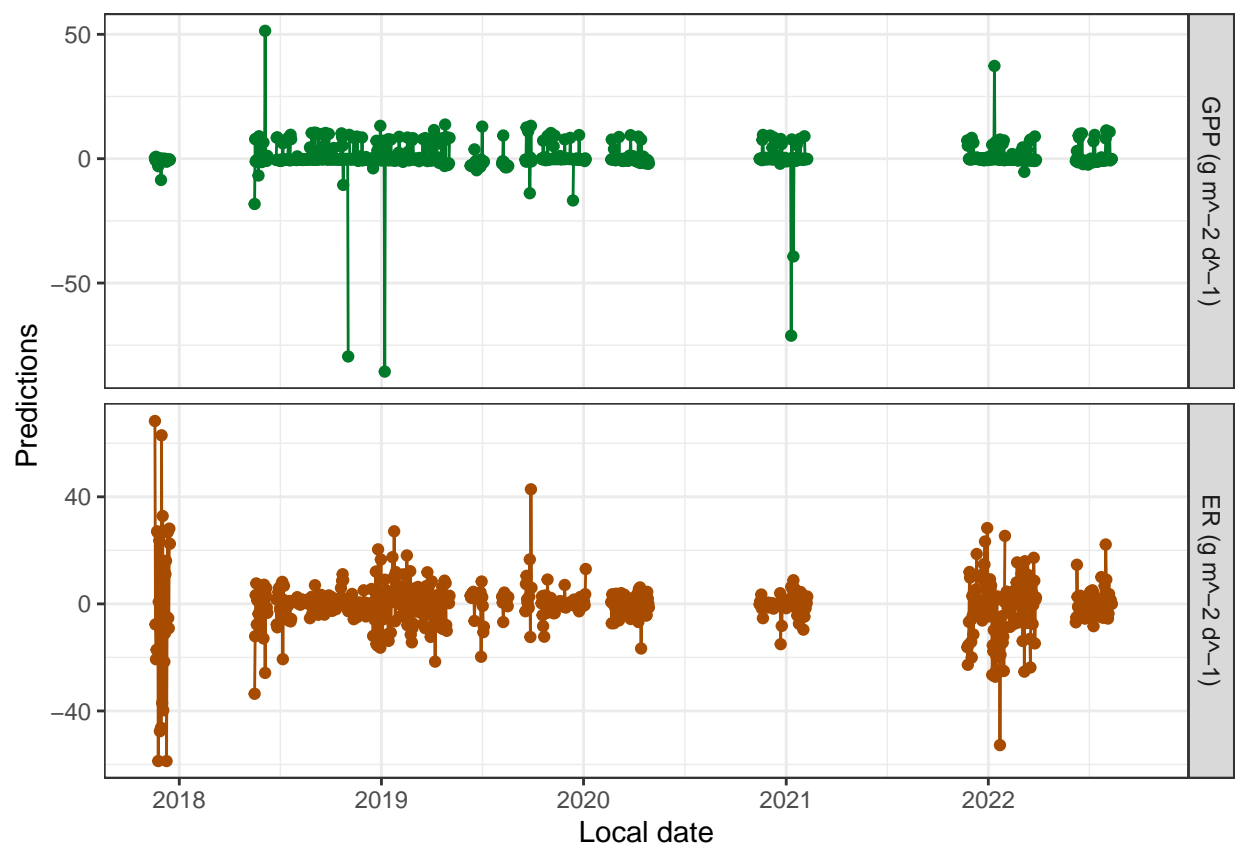
Figure 2: 'Best' model fit.

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 GPP̃light relationship. Saturating models (e.g., 'mm1sat') assume a saturating GPPlight relationship. Lastly, Q10 models (e.g., 'mm1satq10') assume a saturating function of GPP̃light 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.

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mm1_sat	raw	1.6500e+00	170	271	85968.017	-0.603	92.180
mm1_satq10	raw	1.6700e+00	180	281	245690.171	-0.260	745.243
mm5	night	2.5025e+41	574	439	0.936	NA	58.684

ᵃ GPPmean = g C m-2 y-1

lowGPP	lowGPPperc	highGPP	highGPPperc	NAs
840	53.03	30	1.894	1250

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

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	1.6500e+00	170	271	85968.017	-0.603	92.180	0.0000e+00	0.502
mm1_satq10	raw	1.6700e+00	180	281	245690.171	-0.260	745.243	-2.0000e-02	0.498
mm5	night	2.5025e+41	574	439	0.936	NA	58.684	-2.5025e+41	0.000