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Biogeosciences Discussions

Interactive comment on "Optimal Inverse Estimation of Ecosystem Parameters from Observations of Carbon and Energy Fluxes" *by* Debsunder Dutta et al.

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Response to Reviewer 3, Peter Rayner's Comments

This paper demonstrates a method for assimilating site-level flux observations into a terrestrial biosphere model. Its novelty lies in breaking the assimilation into short windows to capture high-frequency variations in the parameters it estimates. given the variety of journals within the Copernicus family, I wonder whether this article is better suited to GMD than BG (see comments below) but this is mainly a question for the editor. The paper is also clearly written, verging on the tutorial at times.

I have one significant concern with the paper and one general request for more analysis. My concern is the analysis of the results. This is quite thin. The only commentary I can see on the results in the discussion section is: "There is strong evidence from measurements that under normal conditions LAI and photosynthetic parameters have seasonal variability [Wang et al., 2008; Wilson and Baldocchi, 2000; Wilson et al., 2000] which correlate with observations of energy fluxes. Our model inversion results are in alignment and agree well with these observations." this seems quite a poor scientific return from a difficult and well-executed piece of work. I would recommend particularly using the posterior simulation to look at some other observables. Do you do a better job matching the high SIF values over the corn site? If so, why, e.g. which parameter, Vcmax or LAI is mainly responsible? What temporal resolution of the parameters is necessary to capture the important variations? I suspect these questions only scratch the surface. I stress that this is potentially a good paper. What it does it does well but I believe it needs more scientific content before publication. If the authors wish to maintain it near its present form I believe it is better suited as a demonstration of a new methodology and hence to GMD.

My request is to delve a little deeper into why the system works better at some places than others. I note there seems less analysis of the Niwot Ridge results which were, in general, also less successful (lower correlation for example). Remember that a less successful assimilation is *not* a failure but rather a useful probe into model performance. It says definitively "we have a problem here and it isn't the choice of parameters". This is even clearer in this case where the parameters are allowed to vary in time.

We thank Peter Rayner for his valuable and insightful comments. These comments have helped us to improve our manuscript greatly. We have addressed the concerns raised and made major revisions to the manuscript following the comments of all the reviewers. We would like to publish this work in Biogeosciences as we think that BG will be a great outlet for readers interested in the coupled carbon and water dynamics

in ecosystems. The developed moving window inversion framework would serve as a valuable tool for the exploration of different and rather difficult to measure ecosystem parameters using a number of observational data streams, this study is an initial step towards this. Moreover, the SCOPE model, which is in the core of inversion framework is also published in Biogeosciences. We thus hope that this journal is appropriate, especially given our substantial improvements in the revised version.

We have added significantly more analysis to the manuscript. We have now incorporated MODIS spectral reflectance bands in the inversion framework for two of our examples. The results are promising and suggest much better constraint on LAI, which in turn reduced fluctuations in Vcmax and BBslope. The retrieved parameters are more realistic and the sensitivity of the inversion towards sudden fluctuations in tower observations is reduced. Within and inter site comparison of the retrievals is also presented when reflectance data is assimilated in the inversion framework.

We have also further added more posterior simulation results and discussed the effect of optimization results for the different sites for different years with and without using MODIS data with flux observations. As suggested we have gone deeper to better explain retrieval results and their fluctuations from the simulations. Discussion about effects of nitrogen variability and Rubisco allocation on Vcmax seasonal variability is also presented. We have also analyzed the results of posterior simulations from Niwot ridge as suggested. Further, we have streamlined our work by moving some material to the supplementary information.

Minor comments P14 In fact the Jacobian doesn't quite show the problem is non-linear, it could be that all the variation is a result of different forcing.

We would like to clarify that the Jacobian shows the response slope at different times of the day due to a small perturbation in the variables of the state vector. Most importantly, we find the Jacobian to changes with subsequent iterations, which is a clear sign of non-linearity.

P16L3 The choice of observational error is quite important in DA, hopefully this is checked later.

Yes, we have included the observational error in the inversion scheme. We assume that the flux observations have uncertainty of 10%. The actual uncertainty of flux observations is hard to characterize and also not available readily, which is why we have made this simplified assumption. The surface energy balance closure error has been generally reported to be around 10-30% (Wilson et. al, 2002, Von Randow et. al, 2004, Sanchez et. al 2010) and is found to be dependent on time-scales due to differences in energy storage terms in ecosystems (Reed, et. al 2018). However, the important point we demonstrate here is the feasibility of the approach in parameter retrieval with full posterior error characterization using suitable a-priori uncertainties. We have included some discussion to state this point and the scope of characterizing the observation noise better in the framework.

Reed, David E., et al. "Time dependency of eddy covariance site energy balance." Agricultural and Forest Meteorology 249 (2018): 467-478.

Wilson, Kell, et al. "Energy balance closure at FLUXNET sites." Agricultural and Forest Meteorology 113.1 (2002): 223-243.

Sánchez, J. M., V. Caselles, and E. M. Rubio. "Analysis of the energy balance closure over a FLUXNET boreal forest in Finland." Hydrology and Earth System Sciences 14.8 (2010): 1487-1497.

von Randow, Coauthors, et al. "Comparative measurements and seasonal variations in energy and carbon exchange over forest and pasture in South West Amazonia." Theoretical and Applied Climatology 78.1-3 (2004): 5-26.

P16L10 I doubt the size of observational vector has much impact on computational efficiency, can you comment why it would?

Thanks for the comment, by size of the observational vector we meant the number of

days and the number of time points (half hourly/hourly) for constructing the concatenated observation vector. This will have a direct impact because it will increase the number of time points (instances) for the forward model runs this will also increase with the number of parameters. This will significantly increase the computational time.

P16L20 The choice of time resolution is also important and yours seems very short. This is likely to lead to parameters which can vary fairly rapidly in time but which are also quite uncertain as they are constrained by fewer observations. Hopefully you can comment on whether parameters change significantly, i.e outside their uncertainty limits.

Thanks for the comments, we believe that the 3-day window sounds is short but reasonable, as variations in environmental stress can happen on synaptic time-scales. It might eventually be better to group the season into blocks with similar "drivers", e.g. VPD, temperature, PAR, but for now, we tried to find a consistent window length, which would allow us to discern short-term fluctuations. We had performed some initial testing with other window sizes (not shown), which showed that a 3-day window is appropriate. Regarding the rapid and abrupt changing of parameters, we could observe this in particular when flux observations appeared to be quite noisy. The addition of more constraint in these cases is extremely beneficial as we have now clearly demonstrated with the inclusion of MODIS reflectance data, which has greatly improved our results for the Mead-1 site. The measure of error reduction has also significantly improved with the inclusion of reflectance data.

P16 Eq. 12, this should have a term from the prior included I think. Unless there's no prior.

Thank you, the full chi-square error we are minimizing in the optimization does have a term from prior error included. However, in order to test the convergence for each iteration in the retrieval windows (and stopping criteria) we use the criterion given in Eq. 12 to test the difference between the fit and measurements (excluding the prior).

This is clarified in the manuscript.

P19L7 "reasonable and realistic" is a little vague, perhaps some references would help.

We agree and have removed this sentence and we have included references in the discussion of results for our examples which support the values of Vcmax and other parameters obtained in this study.

P20L10 be careful about describing correlations as describing how parameters move since these are uncertainty not signal correlations. the sentence above makes it clear you understand this difference but many of your readers will be less clear.

Thank you for this comment/warning. Yes we agree that the error correlation has to be considered as a posterior inversion property and not be confused with actual physical behavior of the variables. These are a result of the inverse retrievals and gives us an indication whether the variable pairs are independent or have a positive or negative association in the retrievals. The actual association in nature between the variables may or may not be similar. We have further clarified this in the manuscript.

P20L14 but here you do confuse signal and error, this correlation does NOT indicate they are changing in sync

We agree the relationship between the variables is only valid in the context of the retrievals and this may or may not be the true association between the variables we find in nature and this association may change depending on different environmental stresses and conditions. We will probably have more confidence regarding the true nature of correlation between the variables if under different retrieval schemes/constraints the error correlations are found to be similar. We are able to include some discussion when we incorporate the MODIS reflectance in the error covariances and compare the error correlations between the two cases. MODIS reflectance data greatly helps to reduce error correlation, in particular between Vcmax and LAI.

P20 in general you seem to be quoting r2 but claim this can be negative. You probably

mean r.

This was also mentioned by the other reviewer, we have now changed all instances in the text and figure to ρ for the correlation coefficient.

P21 I'm not sure that the figures showing your algorithm works are necessary, especially in a journal like biogeosciences where you should focus more on the science and less on the algorithm.

Thank you, we as also mentioned by the other reviewer we have streamlined the presentation and moved some parts to the supplementary information and appendix. We have now moved figure 11 to the appendix as well.

P22L3 as noted earlier the diurnality is not a measure of nonlinearity.

Thank you, as we mentioned we think the variability throughout the day and subsequent evolution when multiple days are concatenated together makes the problem non-linear. In most cases the variability seems diurnal but in some cases K matrix becomes a highly variable and represents a non-linear 3-d surface which varies with different environmental conditions.

P22L10 don't quote improved correlation as a measure of fit, you could have a great correlation and terrible performance if, for example, diurnal variations had great phase and terrible amplitudes. rms is a better though not perfect statistic.

Thank you, we have now presented the coefficient of determination for both prior and posterior simulations for all the examples, together with this we have also now presented the chi2 error statistic as a measure to represent the improvement in performance.

P25 See earlier comments on signal and error correlation.

Thank you, we have again clarified this part in the manuscript.

P25 can you explain further why a strong negative correlation means you need to

optimise both, the step from "you can't see them separately" to "you must do both of them" isn't so clear to me.

Thank you, in this context we simply mean that from the retrieval framework perspective the results indicate there is a strong negative linear association between the two variables. As such these are not independent and therefore not ideal to be optimized independently. We agree that the logic as written was faulty and we have removed this from the text.

P25 I hope you go on to compare the performance at the two sites, one of them seems much harder than the other.

We have now included the MODIS datasets and provided a substantial comparison of the results of parameter retrievals using only flux observations to that using both flux and reflectance observations. The variability in all the three parameters greatly reduced due to the addition of reflectance for the Mead site and at the Ozark site this change made the parameters to be more realistic in addition the posterior simulations suggested a significant improvement in LE fluxes over the other year. These are presented in detail in the revised manuscript.

P27 I'm betting you originally tried to fit LAI at NWR and couldn't. That's not a failure, it's interesting information so is probably worth discussing. You're only fitting in 3 day windows so neither site really knows about the evolution of LAI from one window to the next so why does one work well and the other not, provided I'm guessing correctly.

Thank you, yes this is the unique advantage of using a fully Bayesian framework, we found out approximately the true expected value of LAI for NR and prescribed an extremely low prior error on it and this our windowed simulations maintain it as nearly constant values, this is also a nice test about the mechanism of the inversion. We did some tests where the LAI was allowed to vary and it did indeed trying to match mainly the GPP and LE variability. In terms of physiology the changes in GPP (and LE) in SCOPE is mostly attributed to LAI and Vcmax (and BBslope). In Niwot ridge due to

cold climates there is other plant physiological signaling which stops the photosynthesis without apparent changes in LAI (or Vcmax) like the deciduous forests. This is thus probably a model structural issue which SCOPE is not able to capture just as a stress factor in Vcmax. We have added this part in the NR discussion of results.

P29L13 This site analysis doesn't seem as well developed as the others, e.g. quality of fit etc.

We have now included the results of posterior and prior simulations and discussed the fits after optimizing the parameters.

P29L30 do you mean changes in the temperature dependencies or more simply that there *is* a temperature dependence?

Thank you, we mean changes in temperature dependency due to changes in activation, deactivation and entropy parameters which are incorporated carefully into the modified version of SCOPE in this study and which the current inversion framework is fully equipped to optimize. As discussed this is although a future scope of work.

P30L20 In what sense is the approach "stepwise"? This term was previously used by Bacour et al. (2015), doi:10.1002/2015JG002966) to describe optimising for one observable then using its posterior parameters as priors for the next observable. They would describe your method as "all at once", what do *you* mean by stepwise?

We meant stepwise in the context of a within window optimization, in a sense that the LM algorithm takes a stepwise change in the parameter space taking into account the prior and the observation errors to achieve optimal solutions. As pointed when we look at the broader scheme of things seasonally the optimization seems to be all at once for each time window. We have slightly modified the sentence to better present this.

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