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# *Interactive comment on* "Reconciling differences in stratospheric ozone composites" *by* William T. Ball et al.

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The article deals with the important topic of combining retrieval or composites from several satellite instruments. It nicely illustrates the difficulties in trend estimation with multiple composites having different characteristics. It provides a valid method for constructing a combination of ozone composites from different sources. This a quite general topic. To be able to detect changes in environmental processes, long time series are needed and this in turn leads to need for sound data fusion techniques. Another general topic is that trend analysis crucially depends on realistic uncertainty estimates.

The composites are merged with what the authors call particle filter method. In addition they produce uncertainty estimates for individual composite observation by SVD method. The merged data sets are analysed for trends by using dynamic linear model



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Discussion paper

(DLM) and multiple linear regression (MLR). The article compares the methods and gives recommendations.

As for the recommendations, I agree that DLM is the correct basic framework for analysing time series. It can be seen as a hierarchical Bayesian model or in classical statistical settings, if needed. It has the MLR as a special case, so one can study the need for a "smooth" trend analysis, instead of linear trend. In addition, change points do not have to be prescribed, but their locations can be estimated from the data, and all assumptions can be studies statistically.

I have a couple of general comments about the presentation of the methodology.

**The PF method is presented like a model, but in fact it is a numerical algorithm**

For example
line 17: "Particle filtering and DLM",
line 20: "The particle filter results",
line 779: "using a particle filter",
line 804 "the particle filter as a method".

In my opinion, the distinction between a model for data and a numerical algorithm should be made more clear. You should first describe the model (your dynamical mixture-Gaussian model as a Bayesian hierarchical model) behind the data merge and then the numerical Monte Carlo filtering algorithm (PF/SIR) for actually estimating the merged data set.

PF (or SIR) is a numerical method of computing a certain Monte Carlo estimate of a posterior (predictive) distribution in a dynamical model. You propagate an ensemble ensemble of possible model states (time series realizations) by a model (here the assumed month-to-month seasonal change and known deficiencies) to produce prior ensemble for the next state, which is then weighted by the likelihood function defined by the observed satellite composites. This will form a sample of the posterior uncertainty of the merged series given the observation up to the current time point. In effect this is a non-linear, non-Gaussian generalization of a Kalman filter.

You could contrast this to DLM or MLR "methods". DLM (and MLR, too) is a model for the processes and the system generating the observations (see below for a general state space description. DLM is a structural state space model that constructs a time series from basic building blocks, like trend, seasonality and proxies. For DLM one can use Kalman filter and smoother as an estimation algorithms. For MLR you can use the least squares algorithm for estimation, but other algorithms are available, as well.

**SVD for uncertainty estimates**

A similar comment is valid for the SVD "method" for construction of uncertainty estimates for the individual composites. SVD is an algorithm for a certain matrix decomposition. For the uncertainty analysis, you will have a some kind of model based on principle components and then you use the SVD algorithm for estimating the components. Is there any references the "SVD" approach used? I think the approach would need more motivation. You could write a model for the sources of uncertainties for each composite, having a common source and other sources that might be instrument specific. Then you could estimate these by principle components. As an example, a model for composite $d_i$ would be $d_i = P_i T = p_{1i}T_1 + p_{2i}T_2 + p_{3i}T_3 + p_{4i}T_4$, where $T$ are the principle components and $p$ are the corresponding loadings. Then use it to build a model for variance components of a composite $d_i$, as $\text{var}(d_i) = ...$, that would include the composite uncertainty as one of the components.

**Filter vs. smoother**

You should motivate why "filtering" is adequate for the data merge and no "smoothing" is needed. A filter calculates $p(y_t|\{d_t\})$ for each $t = 1 : T$, but not $p(y_t|\{d_{1:T}\})$ nor the joint distribution $p(y_{1:T}|\{d_{1:T}\})$. The latter are what are estimated by Kalman smoother in DLM calculations for a linear state space model.

Additional question: could PF be replaced by suitable weighted average of the composites, that just takes into account the prior information about problems in the individual series? In DLM and MLR you will need to assume Gaussian uncertainty, so the PF results need to be summarized as mean and standard deviation. What are the benefits of PF over some simpler (non-Monte Carlo) averaging method?

**About MCMC**

I would like to see some MCMC results for the DLM analysis. You are using uniform priors for the variance parameters (line 689). Do these parameter identify, especially, if you assume unconstrained smoothness for the trend? How do the AR parameters identify? You use uniform $[-1, 1]$ for the AR parameter, but do you consider negative autoregression as a realistic model for an ozone observation time series? You could include some plots of the posterior distributions.

**General state space model approach**

I suggest that you describe the merge and trend analyses as a general hierarchical state space model. In both merging the data and in the DLM analysis you are dealing with a dynamical state space model. A general framework to describe the statistical model is by a hierarchical description, with a process model for the model state dynamics, a parameter model for model (nuisance) parameters and a data model for the likelihood. The Bayes formula would provide the posterior estimate from the individual conditional components as (see [1,2,3]):

[process, parameters|data] $\propto$ [data|process,parameters][process|parameters][parameters]

Filtering and smoothing algorithms can be used to estimate various marginal and conditional posterior distributions. The nuisance parameter could be integrated out by MCMC, for example.

For ozone data merge the process model includes the month-to-month variability and external events like volcanos, trends etc. The observation processes could describe the instrument effects. Lastly, there is the prior distributions for model parameters. The whole will in effect be a hierarchical Bayesian model to describe and estimate the state together with the parameters. This could provide a common framework for both merging and analysing.

[1 ] L. M. Berliner. Physical-statistical modeling in geophysics. Journal of Geophysical Research: Atmospheres, 108(D24):8776, 2003. doi: 10.1029/2002JD002865.

[2 ] C. K. Wikle and M. B. Hooten. A general science-based framework for dynamical spatio-temporal models. TEST, 19(3):417–451, 2010. doi: 10.1007/s11749-010-0209-z.

[3 ] N. Cressie and C. K. Wikle. Statistics for Spatio-Temporal Data. Wiley, 2011.

**Other comments**

line 385, equation (2): I do not see how the parameters $\gamma$ and $\beta$ give rise to bimodality for an individual composite as the mean is the same $d_t^c$ for both modes. It probably will make the tails of the likelihood heavier than for a standard Gaussian likelihood.

line 460: The PF distribution is said not to be Gaussian but in DLM and MLR you need Gaussian uncertainty. Is this a problem for the trend analysis?

line 801: "using the same instrument dataset more than once". The transition prior is inferred from the same observations that are used in the model, so the data is used twice. Also, the uncertainty is inferred from the same data by SVD. Maybe this is ok here, but it violates the Bayesian assumptions.

Can you elaborate more the claim that PF method can resolve the problems in data merging? Do you claim that PF is capable to extract the background truth behind different biased estimates. Or does it just make the "error bars" larger, so that the trend analysis is not affected by instrument artefacts?

I agree that construction of a merged data set is of interest in itself. For trend analysis one could start from individual observations. You could discuss the possibility of a general data fusion approach that assimilates all the different composites or individual retrievals to a common time series model. You might still be able to use linear model, but with carefully designed (linear) observation operator, that would account for the instrument artefacts. Or use some non-linear generalization of DLM.

**Conclusion**

I can recommend the article to be published, if the author formulate the modelling approach for merging and uncertainty estimation a little more consistently, motivate the adequacy of the filter in the data merge and the use of SVD for the uncertainty variance components, and describe the MCMC results for DLM.

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