Data Assimilation using an Ensemble of Models: A hierarchical approach

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Abstract. One characteristic of biogeochemical models is uncertainty about their formulation. Data assimilation should take this uncertainty into account. A common approach is to use an ensemble of models. We must assign probabilities not only to the parameters of the models but the models themselves. The method of hierarchical modelling allows us to calculate these probabilities. This paper describes the approach, develops the algebra for the most common case then applies it to the TRANSCOM intercomparison. We see that the discrimination among models is unrealistically strong, due to optimistic assumptions inherent in the underlying inversion. The weighted ensemble means and variances from the hierarchical approach are quite similar to the conventional values because the best model in the ensemble is also quite close to the ensemble mean. The approach can also be used for cross-validation in which some data is held back to test estimates obtained with the rest. We demonstrate this with a test of the TRANSCOM inversions holding back the airborne data. We see a slight decrease in the tropical sink and a notably different preferred order of models.

1 Introduction

Models of any interesting biogeochemical system are inexact. Either they cannot include all interesting processes, the governing equations of processes are not known exactly or computational resolution limits the accuracy of the solution. Throughout this series we stress that quantitative descriptions should be inherently statistical meaning they must include information on the probability of any quantity, either inferred or predicted. This requires us to describe the uncertainty introduced into any quantity by that of the model. Model uncertainty is of two forms, structural and parametric. Structural uncertainties occur when we do not know the functional forms that relate the inputs and outputs of the real system or that control its evolution. In biogeochemical models these functional forms are exactly specified so that uncertainty is usually manifest as an error. Parametric errors occur when the functional forms are well-known but there is uncertainty in various quantities such as constants in physical equations, initial values or boundary conditions. Uncertainties in model predictions arising from parametric uncertainty can be generated by semi-analytic error propagation (e.g. Scholze et al., 2007; Rayner et al., 2011) or by generating ensembles of model simulations from samples of the PDFs of parameters (e.g. Murphy et al., 2007; Bodman et al., 2013).

When structural uncertainty enters the problem only ensemble methods are available. These are usually codified as Model Intercomparison Projects (MIPs) of which the Coupled Model Intercomparison Project (Taylor et al., 2012) for the physical climate and C[4]MIP (Friedlingstein et al., 2006) for the global carbon cycle are prominent examples. The MIPs play a crucial but

controversial role in quantifying uncertainty. First, they may underestimate uncertainty since it is impossible, even in principle, to know how well a given ensemble properly samples the manifold of possible models. On the other hand not all models are equally credible. They do more or less well at tests like fitting observations or conserving required quantities. This has led to the application of Bayesian Model Averaging (e.g. Murphy et al., 2007) in which models are tested against some criteria (such as fit to observations) and their predictions weighted accordingly.

Inverse problems or data assimilation as discussed in this volume generally treats parametric uncertainty. It uses observations and statistical inference to improve knowledge of the uncertain values (see Rayner et al., 2016, and references therein for a general introduction). Structural model uncertainty must still be included and indeed it often dominates other uncertainties. Model uncertainty is hard to characterize with analytic PDFs since errors in the functional forms will project systematically onto errors in simulated quantities. Hierarchical approaches (e.g. Cressie et al., 2009) provide a mechanism for including uncertainties over the choice of model into the formulation. For an ensemble of models this involves introducing an extra discreet variable (the index of the set of models) into the problem and calculating its probability. This probability goes under several names, most commonly the Bayes Factor (Kass and Raftery, 1995). We can then calculate probability distributions for model parameters as weighted averages over these model probabilities. Hence this application of hierarchical Bayesian modelling is closely related to Bayesian Model Averaging (Hoeting et al., 1999; Raftery et al., 2005).

Ensemble methods are rare for biogeochemical data assimilation since there are few problems for which a useful population of assimilation systems currently exists. The clearest exception to this is the case of global scale atmospheric inversions where the TRANSCOM intercomparison (Gurney et al., 2002, 2003, 2004; Baker et al., 2006) used an ensemble of atmospheric transport models and common inversion systems to infer regional CO_2 fluxes from atmospheric concentrations. All these studies faced the problem of estimating properties of the ensemble such as its mean and some measure of spread. Throughout they opted for the ensemble mean and two measures of spread, the standard deviation of the maximum a posteriori (most likely) estimate from each ensemble member and the square-root of the mean of the posterior variances of the ensemble. This treated all members of the ensemble equally.

Equal weighting was challenged by Stephens et al. (2007) who compared the seasonality of vertical gradients in model simulations and observations. They found that only a subset of models produced an acceptable simulation and that this subset favoured larger tropical uptake than the ensemble mean. Pickett-Heaps et al. (2011) compared simulations using optimized fluxes with airborne profiles. This required running optimized fluxes through the forward model used to generate the Jacobians. Of the four models tested TM3 performed substantially better against this extra data than the other three.

Both the cited studies used data not included in the inversion, a procedure often called cross-validation. Cross-validation asks whether new data enhances or reduces our confidence in previous estimates while Bayesian model averaging calculates our relative confidence in two models. We shall see that the machinery needed to answer these two questions is very similar.

The outline of the paper is as follows. In Section 2 we develop the necessary machinery although the detailed algebra is relegated to an appendix. Section 3 describes an application to the TRANSCOM case including an extension to treat covarying model errors. Section 5 discusses the use of the machinery for assessing cross-validation. Section 7 compares the technique with other model evaluation methods as well as discussing some computational aspects.

2 Theory

In traditional data assimilation we do not have a choice over the model relating unknowns to observations. Thus we often forget that the posterior PDFs for unknowns are implicitly dependent on the choice of model. Where an ensemble of models is available we must make this choice explicit. The hierarchical approach factorises this joint PDF of models and unknowns

5 using an expression known variously as the chain rule of probabilities or the law of total probabilities

$$P(x, H_i) = P(x|H_i)P(H_i) \tag{1}$$

$P(x|H_i)$ is the conventional data assimilation problem so the new step is to find $P(H_i)$

We will develop the theory for the simplest linear Gaussian case. Here many of the resulting integrals have analytic solutions. The approach will hold for nonlinear models provided they are approximately linear over enough of the relevant PDFs. The

10 qualitative ranking of models is unlikely to be sensitive to weak nonlinearities since, as we shall see, the discrimination among models is strong.

We follow the notation of Rayner et al. (2016). Take a collection of linear models with Jacobians $\mathbf{H}_1 \ldots \mathbf{H}_N$, with prior estimates of the unknowns defined by the multivariate Gaussian $G(\mathbf{x}^b, \mathbf{B})$ and data defined by the multivariate Gaussian probability $G(\mathbf{y}, \mathbf{R})$.

15 For each $\mathbf{H}_i$ our problem is the simple linear Gaussian inversion described in (Rayner et al., 2016, Section 6.4). Most importantly for us $P(x^a|\mathbf{H}_i)$ is Gaussian. Thus our posterior for the ensemble is a mixture distribution of Gaussians

$$P(\mathbf{x}, \mathbf{H}_i) = W_i G(\mu_i, \mathbf{U}_i) \tag{2}$$

With the constraint that

$$\sum_i W_i = 1 \tag{3}$$

20 The marginal probability for the models is obtained by integrating over $\mathbf{x}$ thus

$$P(\mathbf{H}_i) = W_i \tag{4}$$

and the marginal probability for $\mathbf{x}$ by summing over models:

$$P(\mathbf{x}) = \sum_i W_i G(\mu_i, \mathbf{U}_i)(x) \tag{5}$$

Our problem then is to find W_i. Although the development is probably not novel we derive it in Appendix A for completeness;

25 quoting the result:

$$W_i = K \left| \mathbf{R} + \mathbf{H}_i \mathbf{B} \mathbf{H}_i^T \right|^{-1/2} \exp\left[-\frac{1}{2}(\mathbf{y} - \mathbf{H}_i \mathbf{x}^b)^T \cdot (\mathbf{R} + \mathbf{H}_i \mathbf{B} \mathbf{H}_i^T)^{-1} \cdot (\mathbf{y} - \mathbf{H}_i \mathbf{x}^b) \right] \tag{6}$$

where the normalisation constant K is set such that $\sum_i W_i = 1$. v

2.1 Interpretation

Provided $\mathbf{x}^b$ and $\mathbf{y}$ are independent, $\mathbf{R} + \mathbf{H}_i\mathbf{B}\mathbf{H}_i^T$ is the variance of the prior mismatch $\mathbf{y} - \mathbf{H}_i\mathbf{x}^b$ so Eq. 6 represents the probability of simulating the observations given the prior estimate and related uncertainties. Quite reasonably, the higher this probability the more likely the model. We can say equivalently that the model performance should be judged by the normalised prediction error (simulation − observation divided by its variance) penalised by the expected range of the predictions or the volume of the data space occupied by the prior model and its uncertainty.

Eq. 6 is also the same expression as the maximum likelihood estimate in Michalak et al. (2005). That is reasonable, maximizing the relative probability of a model should mean maximising the Michalak maximum likelihood estimate. It raises the question that relative performance of models may depend strongly on whether the inversion is well-tuned for that model. The algorithm in Michalak et al. (2005) consists of tuning a scaling factor for prior covariances to maximize W_i. We can test the sensitivity to a uniform scaling of $\mathbf{B}$ and $\mathbf{R}$ by a factor α. Increasing α increases the determinant so decreases the first part of W_i while it decreases the negative exponent and so increases the second part. The balance is a relatively subtle change. We will investigate later whether this is enough to change the ranking of models in one example.

The exponent in Eq. 6 is also the minimum value of the cost function usually minimised to solve such systems. It is often denoted $\frac{1}{2}\chi^2$. In a statistically consistent system χ^2 is equal to the number of observations (Tarantola, 1987, P.211). We often quote the normalized χ^2 as $\frac{\chi^2}{[}n]$.

Note also that for a given $\mathbf{B}$ and $\mathbf{R}$, Eq. 6 is extremely punishing on inconsistency. For example with $n = 10000$, a normalized χ^2 of 1.01 instead of 1 yields a ratio of probabilities for the two models of $e^{50} \approx 10^{21}$. This is unrealistic and is an example of the "curse of dimensionality" (Stordal et al., 2011) in which distances between points in high-dimensional spaces tend to infinity. We shall address one approach to resolving this problem later.

2.2 Relationship with Other Criteria

W_i is related to several other measures of model quality. Define

$$\text{JIC} = -2\log(\frac{W_i}{K}) = \log\left|\mathbf{H}_i\mathbf{B}\mathbf{H}_i^T + \mathbf{R}\right| + \chi^2 \tag{7}$$

which we will call Jaynes's Information Criterion after Edwin Jaynes.[1] The change of sign means smaller values of JIC correspond to more likely models. We see that increasing uncertainty of either the prior or the data will decrease χ^2 but increase $\log\left|\mathbf{H}_i\mathbf{B}\mathbf{H}_i^T + \mathbf{R}\right|$.

The JIC is related to Schwarz's Bayesian Information Criterion (BIC) (Schwarz, 1978) which penalizes models for adding parameters. Instead of the term $\log\left|\mathbf{H}_i\mathbf{B}\mathbf{H}_i^T + \mathbf{R}\right|$ the BIC contains the number of parameters n. We note that if we replace $\mathbf{H}_i\mathbf{B}\mathbf{H}_i^T + \mathbf{R}$ with an identity matrix we obtain Schwarz's criterion. The BIC takes no account of different prior uncertainties among parameters or different sensitivities of the observations to these parameters.

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3 The TRANSCOM Example

The **TRANSCOM** III intercomparison (Gurney et al., 2002, 2004; Baker et al., 2006) used a series of atmospheric transport models, represented by matrices of Green's functions, to estimate sources and uncertainties with all other aspects held constant. The authors then created pooled estimates of these quantities such as the mean estimate, the mean uncertainty (averaging all the uncertainties) and finally the "between model" spread, calculated as the covariance among the individual mean estimates.

In all these calculations we weighted every model equally. An obvious objection is that not all models are equal and that we should weight models by some measure of their quality. Stephens et al. (2007) filtered the models according to whether they fitted some independent data of vertical profiles. Pickett-Heaps et al. (2011) also tested their source estimates against independent data. Neither paper, however, took account of the residual uncertainty in the sources. Even if a given inversion didn't fit a profile, was it possible to vary the sources within the uncertainties allowed by the inversion to still fit the profile along with the original surface data?

As a first test of the theory developed in Section 2 we calculate the probability distribution for the models used in the **TRANSCOM** III Level 1 experiment (Gurney et al., 2002). This experiment inverted the annual mean distribution of CO_2 concentrations using 17 different atmospheric transport models.

Figure 1 shows the JIC for the seventeen models for the cases without (top) and with (middle) tuning following Michalak et al. (2005). For the tuning cases we used one multiplier each for the **P** and **R**. We see a large range of weights, 11 orders of magnitude for the untuned and 14 orders of magnitude for the tuned cases. This certainly reflects the "curse of dimensionality" mentioned earlier. For the same reason there is a strong focus of weight on a few models. Tuning intensifies this focus though it leaves the ranking almost unchanged. We conclude therefore that variation in model performance (as measured by the JIC) do not reflect the quality of tuning of the inversion but something more fundamental about the models and data. Henceforth we consider only the untuned case.

Once we have calculated the Gaussian weights we have described the PDF of a joint manifold over the spaces of models and physical parameters. By calculating marginal probabilities from this PDF we can make statements about models or parameters separately.

3.1 Model Probabilities: Comparing Model Performance

The Gaussian weights derived in Section 2 are the probabilities that a given model is the correct one for matching the data under the very strong assumption that we must choose one (the theory does not include a "reject all" option). We must, however, be careful not to over-interpret these probabilities as measures of model quality. In the first place, the JIC, like the BIC and χ^2 grows with the number of observations. So, then, does the divergence among models, an effect intensified when we take exponentials to calculate probabilities. We don't believe that the relative quality of two models depends on the amount of data used to compare them even if our ability to distinguish between them does increase as we add data. We can consider the normalised JIC JIC/N (where N is the number of observations) as a generalisation of the normalised χ^2. This ranges from a minimum of 0.01 to 0.67. The very low value should not be interpreted as representing an absolute quality of fit since we
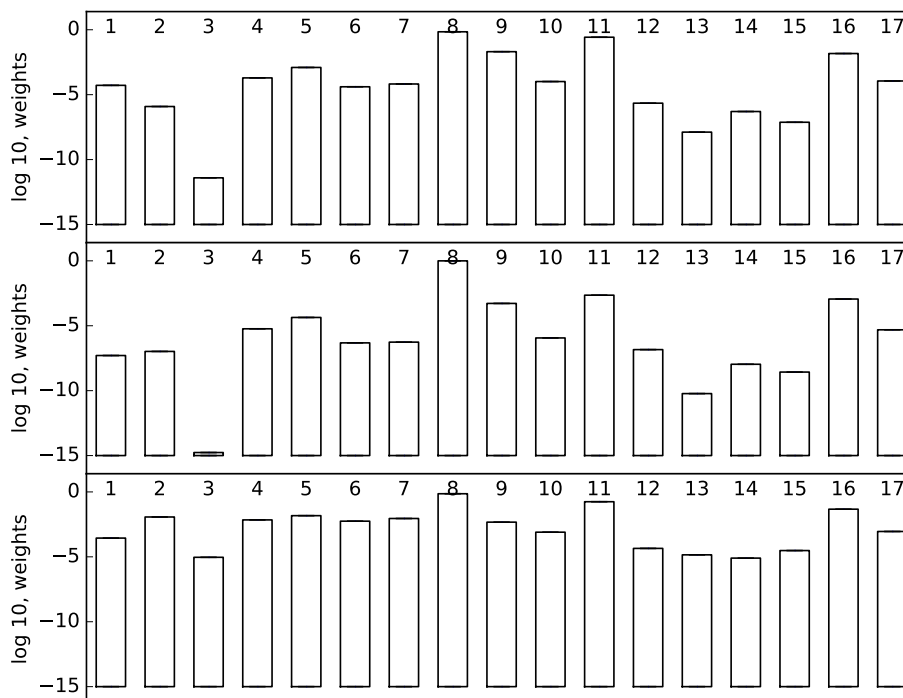
Figure 1. $\log_{10}$ of w_i for the untuned (top), tuned (middle) and case with residuals used for $\mathbf{R}$ (bottom) transcom inversions.

have normalised the probabilities to sum to 1. Rather it tells us that the apparently large change in the weights is a result of much smaller differences in the relative quality of the fit coupled to large amounts of data.

3.2 Ensemble Means and Variances

We can calculate various statistics of the ensemble using well-known properties of Gaussian mixtures. the mean is calculated as

$$\mu = \sum_i w_i \mu_i \tag{8}$$

Note that this collapses to the conventional mean if all weights are equal. the variance is calculated as

$$\sigma^2 = \sum_i w_i \sigma_i^2 + w_i (\mu_i - \mu)^2 \tag{9}$$

We have used roman font for σ and μ to indicate they are scalars. Equation 9 only accounts for the variance not the covariance of the estimates. The second term in Equation 9 includes the spread of the means for each model. If all the w_i are equal, Equation 9 collapses to the "total uncertainty" metric used by Rayner (2004) to incorporate both the "within" and "between" model uncertainty described in Gurney et al. (2002).
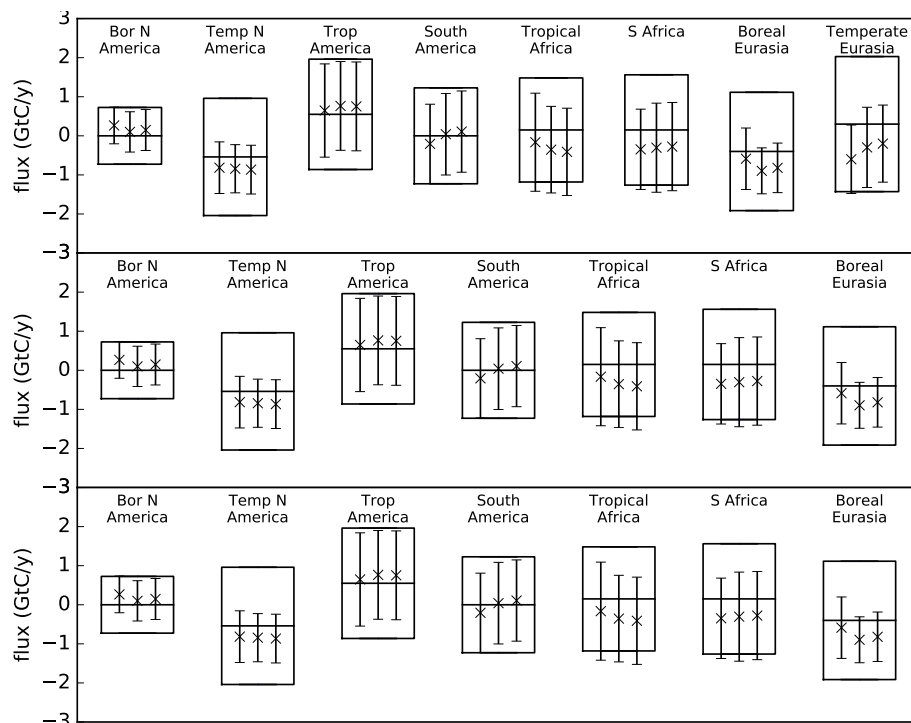
Figure 2. Prior and posterior uncertainties for regional fluxes from the TRANSCOM intercomparison following Gurney et al. (2002). The centre line of each box shows the prior estimate of the mean while the box limits show the $\pm 1\sigma$ uncertainties. The three bars show the mean (marked with "x") and $\pm 1\sigma$ uncertainty denoted by the length of the bar. The uncertainty is that of the ensemble including both the uncertainty for each model and the dispersion among model means. The left bar shows the equally weighted case, the middle bar the case for the w_i and the right bar the case with covariance of residuals included.

Figure 2 shows the equally-weighted and JIC-weighted case for the **TRANSCOM** regions, in a format following Gurney et al. (2002). Here we do not show the "within" and "between" metrics separately since the Gaussian mixture naturally combines them. The focus of w_i on a few models (70% on one model) might suggest that the uncertainty in the weighted case should be far smaller than the equally weighted traditional case. Figure 2 shows this is not the case. Both the means and
5 uncertainties for the two cases are quite similar.

The agreement of the means is explained by a result from Gurney et al. (2002). They noted that the mean simulation from their equally-weighted ensemble produces a better match to the data than any individual model . The JIC-weighted flux is constructed to maximize the posterior probability across the model ensemble and parameter PDFs thus its mean should also produce a good match. It is hence no surprise that the preferred model seven is the model closest to the unweighted model mean.
10 Recalling that the ensemble weights this preferred model at 70% we see good agreement between weighted and unweighted means.

The similarity in the weighted and unweighted total uncertainty is partly a result of the weak data constraint in our problem. Gurney et al. (2002) noted that for almost all regions the "within" uncertainty was larger than the "between". Furthermore the posterior uncertainties produced by each model are rather similar so that the weighted and unweighted contributions in equation 9 are similar. The contributions of the "between" uncertainty are different in the weighted and unweighted cases but,

5   since these are smaller than the other contribution, we do not see a large final difference. This would change in cases where the constraint afforded by the data (as evidenced by the uncertainty reduction cf the prior) was large.

4   Improved Treatment of Observational Covariance

Although mathematically correct, the strong discrimination among models of the JIC is not intuitively reasonable. One reason for the strength of the discrimination is that each datapoint makes an independent contribution to the PDF. This is not an

10   error in the formulation of the JIC but rather the PDF associated with the data in the underlying assimilation.[2] Physically this asumption says that if a model makes an error at one station, one cannot assume it will make a similar error at a nearby station. The physical coherence of atmospheric transport processes makes this most unlikely, even if subgrid heterogeneity lends some independence to the two stations.

There is little machinery available for assigning, a priori, uncertainty correlations for the model. Lauvaux et al. (2009)

15   described a mechanism for calculating correlations due to correlated meteorological uncertainty but this is not a comprehensive description. Thus we are forced to fall back on analysis of the posterior residuals. This technique was previously employed by Kuppel et al. (2013) who derived various aspects of the model contribution to the statistics of the model-data mismatch using techniques described by Desroziers et al. (2005). Desroziers et al. (2005) noted that the residuals must be consistent with the PDF assumed for the model-data mismatch, here described by $\mathbf{R}$. If this is not the case we can make an ad hoc correction to $\mathbf{R}$

20   to include the ensemble covariance of the residuals calculated as

$$\mathbf{R}_{i,j}^{\text{sample}} = \overline{(\mathbf{Hx}_i^{\text{a}} - \mathbf{y}_i)(\mathbf{Hx}_j - \mathbf{y}_j)} \qquad (10)$$

where the overbar denotes an average over the ensemble of models and their respective analyses and the indices i and j refer to observations. Descriptively $\mathbf{R}^{\text{sample}}$ will be positive if, on average, models make errors of the same sign for observations i and j. Note that if the ensemble of models is smaller than the number of observations (usually the case) then $\mathbf{R}^{\text{sample}}$ is singular.

25   This is one reason why we sum $\mathbf{R}$ and $\mathbf{R}^{\text{sample}}$, the other being that the residuals do not capture all the data uncertainty. We note in advance an objection that, by using the residuals, we are double counting information in any subsequent inversion. This is partly true although firstly we only use it to correct the spread not the location of the related PDFs and that the same objection holds for any use of posterior diagnostics.

The weights for the case considering covariance of residuals is shown as the bottom row in Figure 1 and the impact on

30   regional estimates is shown as the right bar in Figure 2. The ranking is similar to the other cases, especially for the preferred models. The main effect of including the residual covariance is to reduce the penalty for the least preferred models. Given

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[2]Strictly speaking it is the model PDF from Rayner et al. (2016), but we have combined model and data uncertainties following their Section 6.4

the small changes among the preferred models it is no surprise that there is little change in the regional estimates or total uncertainties. One reason for the largest impact falling on the least preferred models is that the residual covariance is dominated by the largest residuals which come from the least preferred models.

5   Model Comparison and Cross-Validation

5   In Section 3 we applied the theory to the simplest possible case of models with identical dimensionality and uncertainties; they differed only in their Green's Function. The theory is more general than this. We noted in Section 2.1 that model performance is determined by the normalised prediction error and the volume of the data space occupied by the prior model. Neither of these depends directly on the dimensionality of the prior model. We can compare a model with two highly uncertain parameters against another with four more certain parameters. This extends the BIC which considers only the number of parameters.

10   The case is quite common in biogeochemistry in which we often compare simple models with empirical and highly uncertain parameters with complex, physically-based models whose parameters can be linked to field experiments.

A special case occurs when we compare the prior and posterior models. This is usually done by holding back a subset of the data and testing the improvement in the fit to that data (e.g. Peylin et al., 2016). The approach is frequently called cross-validation. The JIC provides a good basis for comparison of the prior and posterior models. Most importantly it accounts for

15   the different volumes in the data space occupied by the prior and posterior models. Posterior models (informed by the previous assimilation) always occupy less volume in the space of the cross-validation data than their unconstrained or free-running prior model. Thus a good fit to the cross-validation data is less likely to be a chance event.

It is also possible to weight model estimates by their ability to fit cross-validation data. The steps are as follows:

1. Divide data into assimilation and validation data;

20   2. Carry out an ensemble of assimilations using each model and the assimilation data;

3. Calculate the JIC using the *posterior* estimates from step two and the validation data;

4. Calculate ensemble statistics from the posterior estimates from step two and the JIC from step three.

Note that the prior means and covariances in Equation 6 for step three are the posterior means and covariances from step two. Thus, while in Section 3.1 we varied only the model $\mathbf{H}$ here we also vary X^{b} and $\mathbf{B}$. Variations in $\mathbf{B}$ or, more generally,

25   variations in the projection of prior uncertainty into observation space are not usually treated in cross-validation studies (e.g. Pickett-Heaps et al., 2011).

For our example we parallel the test of Stephens et al. (2007). They held back data from airborne profiles and rated models according to their ability to fit seasonal changes in vertical gradients. We cannot use the same measure in our annual mean experiment but we do use the nine points from the airborne profiles above Cape Grim Tasmania or Colorado USA.

30   We can calculate the JIC using these nine measurements and the prior and posterior models. The comparison of the unnormalised JIC for these cases shows whether the fit to the data held back from the inversion has improved. One would hope so
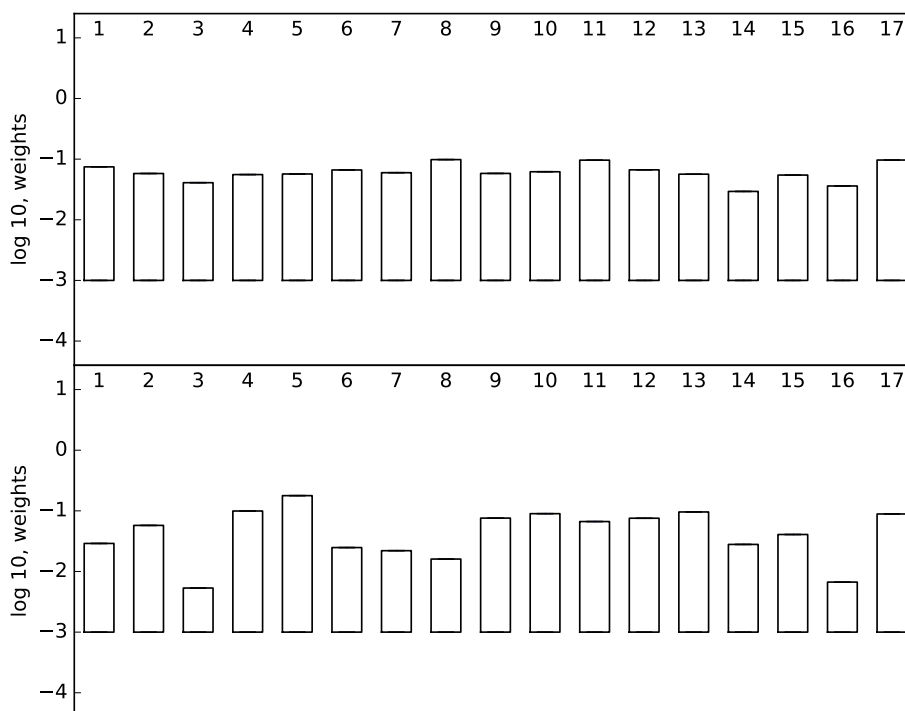
Figure 3. $\log_{10}$ of w_i for the prior (top) posterior (bottom) with the JIC calculated using nine airborne measurements over Cape Grim and Colorado.

but Peylin et al. (2016) showed that this is not always the case. In our case the unnormalised JIC improves by several orders of magnitude due both to a reduction in the residuals and a narrowing of the PDF. Figure 3 shows the comparison of the normalised JIC for the prior (top) and posterior (bottom) models. The prior case shows little variation around the equally-weighted value of $\frac{1}{17}$ while this variation is considerably increased for the posterior case. Figure 4 shows the ensemble statistics for three inversion cases. The left bar is the equally weighted case for the entire network (the left bar from Figure 2), the middle bar shows the equally weighted case for the inversion with the nine cross-validation stations removed while the right bar shows the same inversion but weighted according to the JIC from the cross-validation data. Averaged across all regions the impact of changing network and changing weighting are comparable although the largest changes are in North and South America following from the change of network. This was also observed by Pickett-Heaps et al. (2011).

6 Computational Aspects

The hardest part of the calculation of the JIC is calculating the matrix $\mathbf{HBH}^T + \mathbf{R}$. There are several possible routes depending on the size of the problem and the available machinery. In problems with few parameters it may be possible to calculate and store $\mathbf{H}$ directly. Recall that $\mathbf{H} = \nabla_{\mathbf{x}}\mathbf{y}$. We can calculate $\mathbf{H}$ either as the tangent linear of M (Griewank, 2000) or via finite
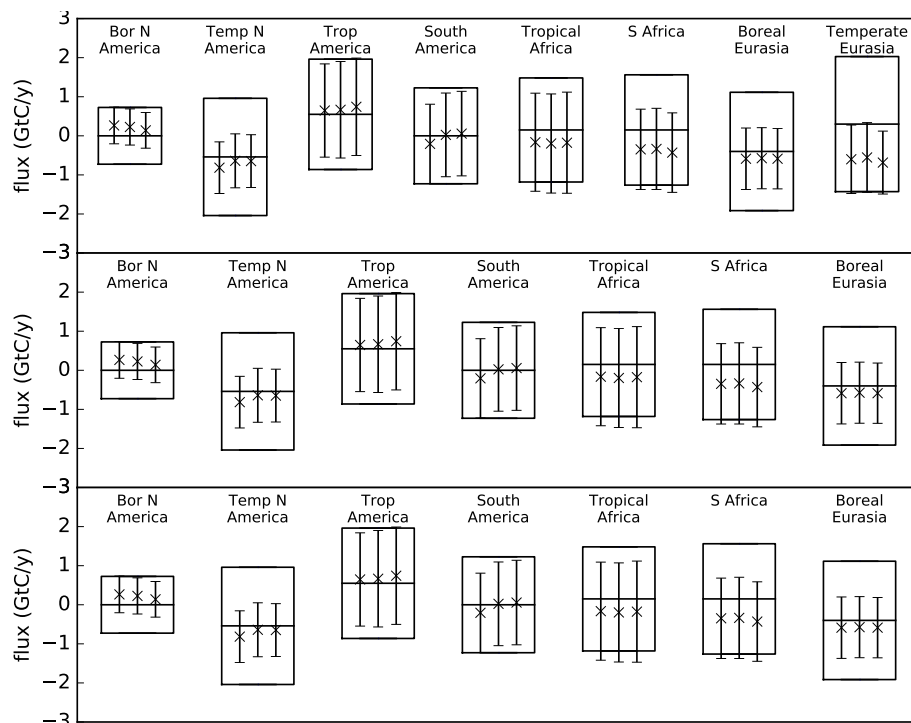
Figure 4. Prior and posterior uncertainties for regional fluxes from the TRANSCOM intercomparison following Gurney et al. (2002). The centre line of each box shows the prior estimate of the mean while the box limits show the $\pm 1\sigma$ uncertainties. The three bars show the mean (marked with "x") and $\pm 1\sigma$ uncertainty denoted by the length of the bar. The uncertainty is that of the ensemble including both the uncertainty for each model and the dispersion among model means. The left bar shows the equally weighted case for the full network, the middle bar the equally weighted case with the cross-validation stations removed and the right bar the JIC-weighted case for the cross-validation data.

difference calculations in which a parameter is perturbed. Once we calculate $\mathbf{H}$ we can generate the eigen-values of $\mathbf{HBH}^T + \mathbf{R}$ from the singular values of $\mathbf{H}$.

If the problem is too large or the generation of the Jacobian too costly we need to generate an approximation to $\mathbf{HBH}^T + \mathbf{R}$ by calculating eigen-vectors from the tangent linear model for $\mathbf{H}$. This is similar to calculations performed in the solution
5 of the assimilation problem itself (Fisher, 1998). The second term in Equation 6 is the Bayesian least squares cost function evaluated at the minimum so, provided we want to calculate X^{a} and not just $P(\mathbf{H}_i)$ we already have this value.

7   Discussion and Future Work

The method we have outlined points out one way of incorporating measures of model quality into ensemble estimates. The TRANSCOM case points out its main limitation, a strong dependence on the underlying PDFs. The same limitation holds for
10 other calculations with the underlying PDFs, especially measures of information content or posterior uncertainty. In cases like

numerical weather prediction where we have repeat assimilations we can easily test that the underlying PDFs are consistent with their realisations but we also have more direct tests of the quality of the assimilation via forecast skill.

A more immediate application than properly weighting an ensemble of models may well be in development where we need to test whether the extra complexity of one version is worth the effort.

8 Conclusions

We have developed a simple application of hierarchical data assimilation to incorporate choice among an ensemble of models. We have demonstrated it for a computationally simple case, the annual mean version of the TRANSCOM intercomparison. The method provides unrealistically strong discrimination among models, mainly due to incorrect assumptions about underlying PDFs. We have also successfully applied the technique to the cross-validation of the TRANSCOM inversions by holding back airborne data over Tasmania and Colorado. The method, when coupled with more sophisticated diagnostics of model-data mismatch should prove a useful extension to traditional biogeochemical data assimilation.

Code and Data Availability

The code and data files to run the TRANSCOM example and generate the figures in the paper can be found at https://figshare.com/articles/Code_needed_to_run_the_transcom_ensemble_weighted_probability_case_for_Data_Assimilation_using_an_Ensemble_of_Models_A_hierarchical_approach_Geoscience_Model_Development_Discussions_2016_w_draft_item/4210212

Appendix A: Appendix A: Finding the Weights

We proceed via the multiplication of PDFs described in (Rayner et al., 2016, Section 4). We start with a uniform prior distribution for the choice of our N models $K(\mathbf{H}_i) = \frac{1}{N}$ and Gaussian PDFs for prior estimates of parameters and for data. Our problem consists of finding the marginal probability $P(\mathbf{H} = \mathbf{H}_i)$.

Using Eq. 1.93 from Tarantola (2005) we have

$$p(\mathbf{H}_i, \mathbf{x}) = \frac{K(\mathbf{H}_i)G(\mathbf{x}, \mathbf{x}^{\mathrm{b}}, \mathbf{P}) \cdot G(\mathbf{H}_i\mathbf{x}, \mathbf{y}, \mathbf{R})}{\sum_i \int K(\mathbf{H}_i)G(\mathbf{x}, \mathbf{x}^{\mathrm{b}}, \mathbf{P})G(\mathbf{H}_i\mathbf{x}, \mathbf{y}, \mathbf{R})dx} \tag{A1}$$

We wish to find

$$P(\mathbf{H} = \mathbf{H}_i) = \int \sigma(\mathbf{H}_i, \mathbf{x})dx \tag{A2}$$

and also

$$P(\mathbf{x}) = \sum_i p(\mathbf{x}, \mathbf{H}_i) \tag{A3}$$

A0.1 Model Probability

the denominator is a normalization so if we worry only about relative likelihoods we need only the integral of the numerator.
The multivariate Gaussian can be expanded as:

$$G(\mathbf{x}\mu, \mathbf{C}) = (2\pi)^{-n/2} |\mathbf{C}|^{-1/2} \exp\left[-\frac{1}{2}(\mathbf{x}-\mu)^T \cdot \mathbf{C}^{-1} \cdot (\mathbf{x}-\mu)\right] \tag{A4}$$

where n is the dimension of μ.

Substituting Eq. A4 into Eq. A1 gives

$$p(\mathbf{H}_i, \mathbf{x}) \propto |\mathbf{P}|^{-1/2} |\mathbf{R}|^{-1/2} \exp\left[-\frac{1}{2}(\mathbf{x}-\mathbf{x}^b)^T \cdot \mathbf{P}^{-1} \cdot (\mathbf{x}-\mathbf{x}^b)\right] \exp\left[-\frac{1}{2}(\mathbf{H}\mathbf{x}-\mathbf{y})^T \cdot \mathbf{R}^{-1} \cdot (\mathbf{H}\mathbf{x}-\mathbf{y})\right] \tag{A5}$$

To simplify this expression we note that determinant is distributive over multiplication and also that multiplying exponentials is achieved by adding exponents. Some linear algebra, completing the square and the use of the special form of the matrix inversion lemma

$$(\mathbf{P}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1} = \mathbf{P} - \mathbf{P}\mathbf{H}^T(\mathbf{H}\mathbf{P}\mathbf{H}^T + \mathbf{R})^{-1}\mathbf{H}\mathbf{P} \tag{A6}$$

we can reduce Eq. A5 to the form

$$p(\mathbf{H}_i, \mathbf{x}) \propto |\mathbf{P}|^{-1/2} |\mathbf{R}|^{-1/2} \exp\left[-\frac{1}{2}(\mathbf{x}-\mu)^T \cdot \mathbf{A}^{-1} \cdot (\mathbf{x}-\mu)\right] \times \exp\left[-\frac{1}{2}(\mathbf{y}-\mathbf{H}_i\mathbf{x}^b)^T \cdot (\mathbf{R}+\mathbf{H}_i\,mathbf{P}\mathbf{H}_i^T)^{-1} \cdot (\mathbf{y}-\mathbf{H}_i\mathbf{x}^b)\right] \tag{A7}$$

where

$$\mu = \mathbf{x}^b + \mathbf{P}\mathbf{H}_i^T \cdot (\mathbf{R}+\mathbf{H}_i\mathbf{P}\mathbf{H}_i^T)^{-1} \cdot (\mathbf{y}-\mathbf{H}_i\mathbf{x}^b) \tag{A8}$$

and

$$\mathbf{A}^{-1} = \mathbf{P}^{-1} + \mathbf{H}_i^T\mathbf{R}^{-1}\mathbf{H}_i \tag{A9}$$

Note that Eqs. A8 and A9 are the standard expressions for the posterior mean and variance of $mathbf{x}$. Now substituting in Eq. A2 and using the fact that

$$\int d\mathbf{x} \exp\left[-\frac{1}{2}(\mathbf{x}-\mu)^T \cdot \mathbf{A}^{-1} \cdot (\mathbf{x}-\mu)\right] = |\mathbf{A}|^{1/2}(2\pi)^{n/2}$$

we have

$$p(\mathbf{H}_i) \propto |\mathbf{A}\mathbf{P}^{-1}| |\mathbf{R}^{-1}| \exp\left[-\frac{1}{2}(\mathbf{y}-\mathbf{H}_i\mathbf{x}^b)^T \cdot (\mathbf{R}+\mathbf{H}_i\mathbf{P}\mathbf{H}^T)^{-1} \cdot (\mathbf{y}-\mathbf{H}_i\mathbf{x}^b)\right] \tag{A10}$$

We also have the condition that

$$\sum_i p(\mathbf{H}_i) = 1. \tag{A11}$$

Finally we can simplify $\left| \mathbf{A}\mathbf{P}^{-1} \right|\left| \mathbf{R}^{-1} \right|$ using Eq. A6 and Sylvester's Determinant Theorem which states that for any matrices $\mathbf{U}$ and $\mathbf{V}$

$$|\mathbf{I} + \mathbf{U}\mathbf{V}| = |\mathbf{I} + \mathbf{V}\mathbf{U}| \tag{A12}$$

Substituting and simplifying yields

$$5 \quad p(\mathbf{H}_i) \propto \left| \mathbf{R} + \mathbf{H}_i\mathbf{P}\mathbf{H}_i^{\mathrm{T}} \right|^{-1/2} \exp\left[-\frac{1}{2}(\mathbf{y} - \mathbf{H}_i\mathbf{x}^{\mathrm{b}})^T \cdot (\mathbf{R} + \mathbf{H}_i\mathbf{P}\mathbf{H}_i^T)^{-1} \cdot (\mathbf{y} - \mathbf{H}_i\mathbf{x}^{\mathrm{b}}) \right] \tag{A13}$$

A1

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