

Referee’s Report: “Data Assimilation Using an Ensemble of Models: A Hierarchical Approach” by Peter Rayner, submitted to *Atmospheric Chemistry and Physics*.

This paper considers the structural uncertainty for the inversion problem and applies the Bayesian model averaging methodology (e.g., Raftery et al., 1997; Hoeting et al., 1999) to obtain the posterior ensemble mean and variance of \mathbf{x} for a number of inversion models. Compared with simply assigning equal weights to each inversion model, the method in this paper is statistically more appropriate for obtaining the posterior statistics of the ensemble.

1 Major Comments

1. Some notations in this paper are not very consistent. For example, at the beginning of Section 2, the author used $p(\cdot)$ for probability density function (PDF), but later on $P(\cdot)$ was used for PDF. In addition, for function $H_i(\cdot)$ and matrix \mathbf{H}_i , it is better to add some notes to make a clear distinction. Last, the criterion L in Equation (5) is not italic, but later on it appears in italic font and hence can be a bit confusing.
2. The conditional densities in Equations (1) and (4) are also conditional on \mathbf{x}^b , and hence the author should mention \mathbf{x}^b is omitted for notation simplicity. Besides, is the prior mean \mathbf{x}^b treated as a fixed or random quantity in this paper?
3. Page 4, Line 7, the author mentioned that “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 $\mathbf{y} - \mathbf{H}_i\mathbf{x}^b$...”, which seems to be inappropriate. This is because the matrix \mathbf{B} is the covariance matrix of \mathbf{x} , not of the prior mean \mathbf{x}^b .
4. Page 6, in Figure 1, why the weight of model 3 is so small for the tuned case, compared with other two cases?
5. The author claims that Equation (7) is the variance of the ensemble, which seems to be incorrect. From the formulation, it seems to be the mean squared (prediction) error for \mathbf{x} .
6. Page 7, Figure 2: The titles of boxplots are repeated for each row but it is supposed that the results for all the 22 regions are reported. The author should double check whether this figure is correctly produced.
7. For Equations (8) and (9), it is better to give the mathematical definition of the mean terms (e.g., the mean of $\mathbf{H}(x)_i^b$); also the superscript a is missed in Equation (9). Could the author provide more motivations for using $\mathbf{R}_{i,j}^{\text{prior}}$ and $\mathbf{R}_{i,j}^{\text{sample}}$?
8. Page 9, Line 6: The author pointed out that the residual covariances have the largest values for a few terrestrially-influenced stations such as Baltic Sea and so on. A figure showing the residual covariances can be added to support this claim.
9. Page 10, for the section of computational aspects: Provided that \mathbf{R} is a sparse matrix (e.g., diagonal), I think the computational trick is to use a low-rank matrix to approximate $\mathbf{H}_i\mathbf{B}\mathbf{H}_i^T$; then we can resort to the Sherman-Woodbury-Morrison inversion formula to compute the inverse of $(\mathbf{H}_i\mathbf{B}\mathbf{H}_i^T + \mathbf{R})$ and the Sylvester’s theorem to compute its determinant (e.g, Cressie and Johannesson, 2008; Sang and Huang, 2012). The author may add a bit more details to make the computational strategy more clear.
10. Page 12, Figure 4: Similar to Figure 2, the results seem to be repeated and not all the regions’ statistics are reported. The author should double check whether the figure is correctly produced.

2 Minor Comments

1. Page 1, Line 23, the right bracket should be removed.
2. Page 2, Line 12, “discreet” should be “discrete.”
3. Page 3, Line 2: “the” in “the standard data assimilation...” should be capitalized. Similarly, Page 6, Line 11: “the” in “the variance is calculated as” should be capitalized. The author needs to double check whether there are similar typos in the paper.
4. The author refers the Equation (1) but I do not see Equation (1) in the context.

5. Page 4, in the second and third paragraph, it seems that $P(\mathbf{H}_i)$ should be $P(\mathbf{H}_i|\mathbf{y})$.
6. Page 4, Line 23: "... χ^2 is equal to the number of observations..." should be "... the expected value of χ^2 is equal to the number of observations..."
7. Page 7, Line 1: "The Superscripts * indicates we consider..." should be "The superscript * indicates we consider..."
8. Page 9, Line 6: "Eq. 9 and Eq. 8" should be "Eq. 8 and Eq. 9".
9. Page 10: the math symbols, X^b and X^a should be \mathbf{x}^b and \mathbf{x}^a , respectively.
10. Page 11: in the caption of Figure 3, the author should give the full name of "JIC."

References

- Cressie, N. and G. Johannesson (2008). Fixed rank kriging for very large spatial data sets. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 70, 209–226.
- Hoeting, J. A., D. Madigan, A. E. Raftery, and C. T. Volinsky (1999). Bayesian model averaging: A tutorial. *Statistical Science* 14, 382–401.
- Raftery, A. E., D. Madigan, and J. A. Hoeting (1997). Bayesian model averaging for linear regression models. *Journal of the American Statistical Association* 92, 179–191.
- Sang, H. and J. Huang (2012). A full scale approximation of covariance functions for large spatial data sets. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 74, 111–132.