Computing an Ensemble of Variational Data Assimilation using its Mean and Perturbations

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Abstract:
We show how to reformulate an ensemble of variational data assimilation minimisations by focusing on the ensemble mean first and then the perturbations about the mean. Tests using the Met Office system show that this Mean-Pert method can give practically identical results to minimising each member individually results at much reduced cost. This provides a cost-effective system for hybrid ensemble-variational data assimilation for numerical weather prediction.

Methodology:
For an ensemble of variational data assimilations, for $k=1,...,Nens$, and r_k random observation perturbation, the k-th analysis x_k^a minimises the penalty function

$$J(x_k)=\frac{1}{2}\left(x_k-x_k^b\right)^T B^{-1}\left(x_k-x_k^b\right)+\frac{1}{2}\left[y^{obs}+r_k-H(x_k)\right]^T R^{-1}\left[y^{obs}+r_k-H(x_k)\right],\ k=1,...,Nens.$$

Using the transformed control variable $x_k-x_k^b=Uv_k$, where $B=UU^T$

$$J(v_k)=\frac{1}{2}v_k^T v_k+\frac{1}{2}\left[y^{obs}+r_k-H\left(x_k^b+Uv_k\right)\right]^T R^{-1}\left[y^{obs}+r_k-H\left(x_k^b+Uv_k\right)\right],\ k=1,...,Nens \quad (1)$$

Assuming H is weakly nonlinear $H\left(x_k^b+Uv_k\right)\approx H(x_k^b)+HUv_k,\ \forall\, k=1,...,Nens$ the minimiser v_k^a satisfies

$$\text{(analysis equation)}\quad v_k^a=U^TH^T\left(HBH^T+R\right)^{-1}\left(y^{obs}+r_k-H(x_k^b)\right),\ k=1,...,Nens$$

$$\text{(ensemble mean equation)}\quad \bar{v}^a=U^TH^T\left(HBH^T+R\right)^{-1}\left(y^{obs}-H(\bar{x}^b)\right)$$

$$\text{(perturbation around the mean equation)}\quad v'^a_k=U^TH^T\left(HBH^T+R\right)^{-1}\left(r_k-H(x'^b_k)\right),\ k=1,...,Nens$$

Variationally, $\bar{v}^a$ and v'^a_k are respectively the vectors that minimise the respective penalty functions

$$J(\bar{v})=\frac{1}{2}\bar{v}^T\bar{v}+\frac{1}{2}\left[y^{obs}-H(\bar{x}^b+U\bar{v})\right]^T R^{-1}\left[y^{obs}-H(\bar{x}^b+U\bar{v})\right] \quad (2)$$

$$J(v'_k)=\frac{1}{2}v'^T_k v'_k+\frac{1}{2}\left[r_k-H(x'^b_k+Uv'_k)\right]^T R^{-1}\left[r_k-H(x'^b_k+Uv'_k)\right],\ k=1,...,Nens \quad (3)$$

How to use the Mean-Pert method :

- Since the Met Office data assimilation system is designed to use full fields rather than perturbations in the observation operators, we first find $\bar{v}^a$ by minimizing

$$J(\bar{v})=\frac{1}{2}\bar{v}^T\bar{v}+\frac{1}{2}\left[y^{obs}-H(\bar{x}^b+U\bar{v})\right]^T R^{-1}\left[y^{obs}-H(\bar{x}^b+U\bar{v})\right]$$

- On the final iteration of the minimisation, store the analysed values of the observations $H(\bar{x}^b+U\bar{v})=H(\bar{x}^a)=\bar{y}^a$ and the affine function $\tilde{H}(x)=H(x-\bar{x}^a)+\bar{y}^a$
- We then seek $v_k=v'_k+\bar{v}^a$ that minimizes

$$J(v_k)=\frac{1}{2}(v_k-\bar{v}^a)^T(v_k-\bar{v}^a)+\frac{1}{2}\left[\bar{y}^a+r_k-\tilde{H}(x_k^b+Uv_k)\right]^T R^{-1}\left[\bar{y}^a+r_k-\tilde{H}(x_k^b+Uv_k)\right] \quad (4)$$

How to handle nonlinear H :

Important nonlinearities occur for instance in H for observations affected by humidity when cloud forms, or in the handling of observations with a finite probability of gross error when they are close to rejection Dharssi et al. (1992).
Re-linearising the ensemble mean minimisation of (2) about the current best estimate, the variational methods have the best chance of making correct assumptions about the presence of cloud or the quality of observations. The derivation of (3) and (4), all made assumptions that H is linear.
So although (4) looks as if we could replace $\tilde{\mathrm{H}}$ by H, there is no justification for doing so.
The quality control of observations with non-Gaussian errors can also lead to nonlinear effects . Each member of the control ensemble makes its own decision about the rejection of a borderline observation. The Mean-Pert method makes its decision using the ensemble mean.

Experimental set-up :

The trials run for this work used ensembles of 4DEnVar assimilations; the setup used follows Bowler et al. (2016).

- N216 resolution (432×324 grid-points on a regular latitude-longitude grid) with 70 levels in the vertical going up to 80km
- Hybrid background-error covariances. First experiment, equal weight to the static background-error covariance and ensemble-based background-error covariance. A second experiment used an ensemble of 3DVar with First-Guess at Appropriate Time (FGAT).
- Additive and multiplicative inflations. A blend of the Relaxation-To-Prior Perturbation (RTTP, Zhang et al. (2004)), and the Relaxation-To-Prior Spread (RTPS, Whitaker and Hamill (2012)) was used.
- To control imbalance in the NWP forecasts we use a 4DIAU Lorenc et al. (2015)
- 44 ensemble members.

Results and concluding remarks:
Number of iterations and timings: The major benefit of using the Mean-Pert Ensemble Data Assimilation is the computational time saving. The control experiment used 60 iterations to minimise (1) for each ensemble-member, as does the Mean-Pert when minimising (2) , which is done once. Twenty iterations was judged sufficient for the perturbation minimisations (4) whose rate convergence is shown in figure (1). Because of the data volumes for the ensemble trajectories used by each 4DEnVar, " it is not possible to run 4DEnVar minimisations in parallel on our system, so the total elapsed time is a good measure of cost." I'm working on this ! The Mean-Pert method reduces the cost scale $N_{iter}\times N_{ens}^2$ by doing fewer iterations; in our test by a factor of 3, see figure 2. We also tested the effect of preconditioning using 7 Lanczos eigenvectors and 20 iterations, the results are presented in figure 3. For more details see Lorenc et al. (2016) .

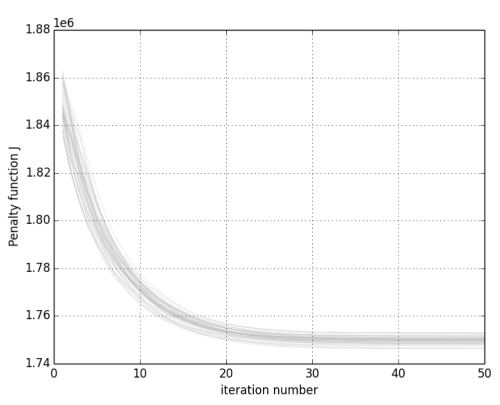

Figure 1

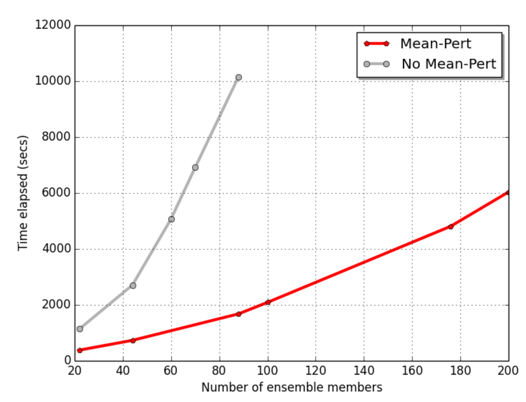

Figure 2

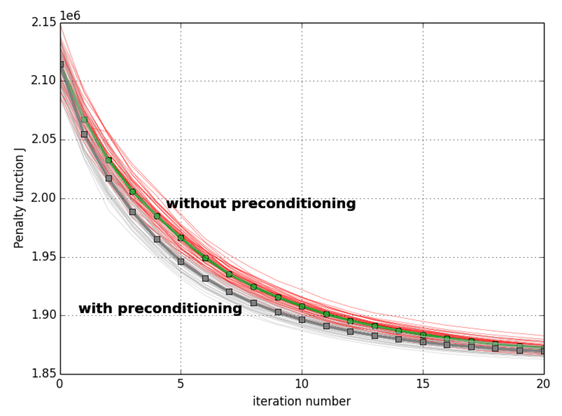

Figure 3

Ensemble validation and verification: Figure 4 compares the ensemble mean analyses at the end of the control and Mean-Pert trials using 44 ensemble members for a period spanning 0000 UTC 24 January 2014 to 0000 UTC14 March 2014. Figure 5 is similar to figure 4 with the ensemble spread replacing the ensemble mean for each of the considered fields. The absolute value of the difference of the considered quantities reveals that qualitatively the Mean-Pert method produces results similar to the fully nonlinear minimisations, but at a lower computational cost.

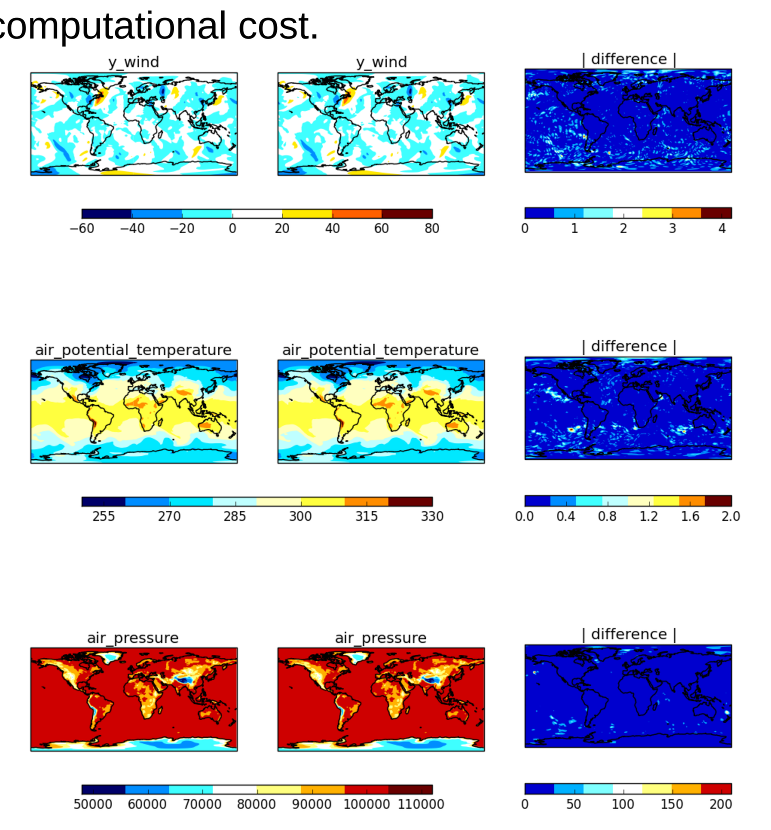

Figure 4

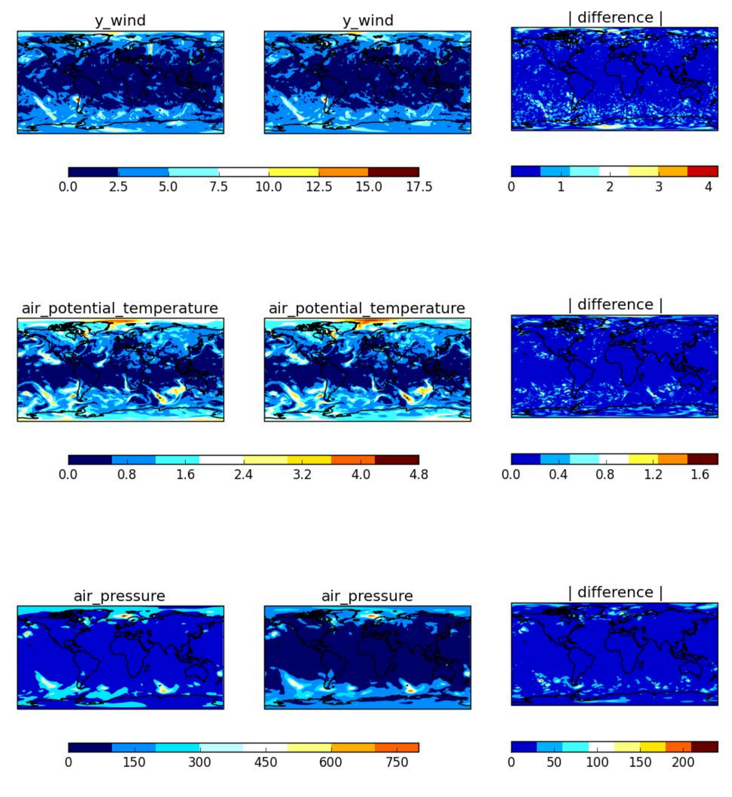

Figure 5

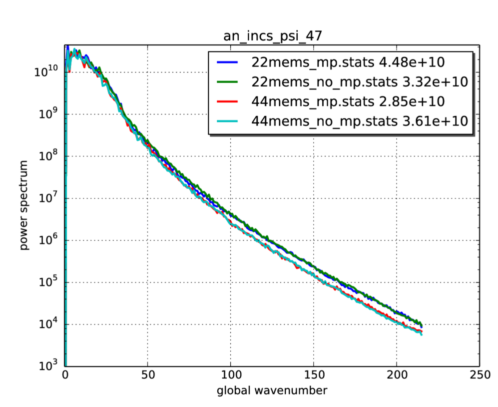

Figure 6

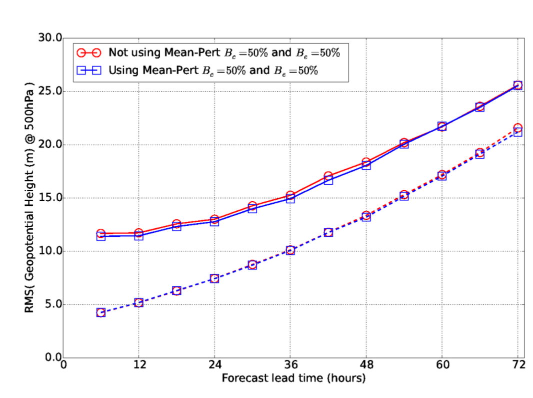

Figure 7

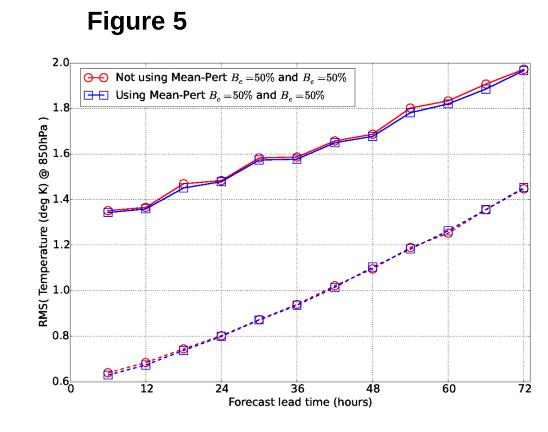

Figure 8

We compared the power spectra of the ensemble analysis increments with and without Mean-Pert; figure 6 shows no significant difference from using the Mean-Pert method. The differences between ensemble verification RMSE and the ensemble spread σ for a 44 ensemble member trial with and without Mean-Pert Are small (figures 7 and 8) .

Concluding remarks:
We have shown that the Mean-Pert method reduces the computational cost od an ensemble of variational data assimilations without significantly altering results. For the experiments presented in Bowler et al.(2016) this reduced the cost of the analysis step by a factor of 3. The method could be applied to ensembles of 4DVar like those described in Raynaud et al.(2011); Bonavita et al.(2016) . In building the most cost-effective hybrid ensemble-variational data assimilation system, other aspects need to be considered. If the ensemble mainly provides error covariance estimates then it is worth devoting more resources to the "best estimate" than to each ensemble-member traditionally NWP centres have used "deterministic" NWP systems run at higher resolution to give the best estimate. Should we replace the ensemble mean in the Mean-Pert method by such a system? In contrast, if the details of each ensemble member are used, for instance in forecasting rare high-impact events, then we may need to change the traditional approaches, based on Gaussian distributions, that are used to verify our forecasts and are the basis of variational DA methods.

References:
Bonavita M, Holm E, Isaksen L, Fisher M. 2016. The evolution of the ECMWF hybrid data assimilation system. Q. J. R. Meteorol.Soc.142(694): 287–303.
Bowler NE, Clayton AC, Jardak M, Lee E, Lorenc AC, Piccolo C, Pring SR, Wlasak MA, Barker DM, Inverarity GW, Swinbank RS. 2016. Inflation and localisation tests in the development of an ensemble of 4D-ensemble variational assimilations Q. J. R. Meteorol. Soc. submitted.
Dharssi I, Lorenc A, Ingleby N. 1992. Treatment of gross errors using maximum probability theory. Q. J. R. Meteorol. Soc.118:1017–1036.
Lorenc AC, Jardak M, Payne T, Bowler NE, Wlasak MA . 2106. Computing an Ensemble of Variational Data Assimilations using its Mean and Perturbations. Q. J. R. Meteorol. Soc. submitted
Raynaud L, Berre L, Desroziers G. 2011. An extended specification of flow-dependent background-error variances in the Météo-France global 4D-Var system.Q. J. R. Meteorol. Soc.137: 607–619.
Whitaker JS, Hamill TM. 2012. Evaluating methods to account for system errors in ensemble data assimilation. Mon. Weather Rev.140: 3078–3089.
Zhang F, Snyder C, Sun J. 2004. Impacts of initial estimate and observation availability on convective-scale data assimilation with an ensemble Kalman filter. Mon. Weather Rev.132(5):1238-1253.

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