P3.11 A COMPARISON OF AN ENSEMBLE OF POSITIVE/NEGATIVE PAIRS AND A CENTERED SPHERICAL SIMPLEX ENSEMBLE

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1 INTRODUCTION

The Ensemble Transform Kalman Filter (ETKF) ensemble generation technique (Wang and Bishop 2003) provides dynamic ensemble perturbations rather than the random sample perturbations. In Wang and Bishop (2003) no explicit method whereby the ensemble perturbations could be centered about the best available estimate of the true state, that is, the control analysis is provided. This is undesirable because, ideally, one would like the ensemble mean to *always* be equal to the minimum error variance estimate of the true state.

The question of how one should center an ensemble does not appear to have received much attention in published literatures. Operationally, the singular vector (SV) scheme (Buizza and Palmer 1995; Molteni et al. 1996) and the breeding scheme (Toth and Kalnay 1993, 1997) both select symmetric positive/negative paired centering, where an ensemble of K initial perturbations (note we define an ensemble as K perturbed members plus one control member) is created by letting half of these perturbations be the negative of the other half. Toth and Kalnay (1997) also raised another method where centered perturbations are obtained by removing the average of the perturbations from each individual perturbation vector. We call it the subtract-mean method.

Besides making the sum of the perturbations equal to zero, there are two more aspects that one needs to control when centering the initial perturbations. First, if the ensemble covariance is going to be used to estimate the forecast error covariance then one would like the covariance of the initial perturbations before and after centering to be preserved; second, if ensemble perturbations are to be treated as equally likely error realizations, then the centered perturbations must be equally likely. The traditional symmetric positive/negative pair method satisfies the above requirements. For the spherical simplex method to be introduced in this paper, one linearly dependent perturbation is added to the one-sided ETKF ensemble to satisfy all these three requirements. The subtract-mean method however does not satisfy all these three requirements (refer to Wang et al. 2003, the complete manuscript for details).

For ensemble size large enough to span *all* uncertain directions, the symmetric positive/negative paired centering that provides 3rd order accurate ensemble mean and ensemble covariance, becomes superior to the spherical simplex centering that only provides 2nd order accuracy. But if the ensemble size is not sufficiently large, which is true for a high dimensional system, the spherical simplex centering can describe error covariance in up to K-1 directions rather than just K/2 directions as in the symmetric positive/negative paired centering. The extent to which the theoretical superiority of one scheme over the other would be born out when K is less than the number of uncertain directions might depend on things like the dominance of the directions spanned by the ensemble and the extent to which the ensemble accounted for model error.

The goal of this paper is to test both centering methods on the ETKF scheme. In section 2 we briefly introduce the mathematical expressions of the spherical simplex ETKF. Section 3 describes how the numerical experiment is designed. Section 4 compares the numerical experiment results of the two centering schemes. In section 5 we summarize the results.

2 THE SPHERICAL SIMPLEX ETKF

Define K forecast perturbations at the 12-h forecast lead-time as,

$$\mathbf{X}^f = (\mathbf{x}_1^f - \overline{\mathbf{x}}^f, \mathbf{x}_2^f - \overline{\mathbf{x}}^f, \cdots, \mathbf{x}_K^f - \overline{\mathbf{x}}^f), \quad (1)$$

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where $\mathbf{x}_i^f$, $i=1,\cdots,K$, are K perturbed 12-h forecasts and $\overline{\mathbf{x}}$ is the mean of the K perturbed 12-h forecasts, i.e.,

$$\overline{\mathbf{x}} = \left(\mathbf{x}_1 + \mathbf{x}_2 + \cdots + \mathbf{x}_K\right)/K. \qquad (2)$$

After postmultiplying (1) by the transformation matrix $\mathbf{T} = \mathbf{C}(\mathbf{\Gamma}+\mathbf{I})^{-1/2}$ (see Bishop et al. 2001 and Wang and Bishop 2003) where $\mathbf{C}$ and $\mathbf{\Gamma}$ are the eigenvector and eigenvalue matrices of $(\mathbf{X}^f)^{\mathrm{T}}\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\mathbf{X}^f/K$ ($\mathbf{H}$ is the observation operator and $\mathbf{R}$ is the observation error covariance matrix), only $K-1$ independent ETKF analysis perturbations are generated. This is because the sum of the *K* forecast perturbations in (1) is zero and therefore the last element of $\mathbf{\Gamma}$ is equal to zero. Thus, (1) postmultiplied by the last column of $\mathbf{C}$ is a zero vector (note the determinant of $\mathbf{H}$ generally is not zero). Mathematically, the $K-1$ one-sided ETKF analysis perturbations are

$$\mathbf{X}^a = (\mathbf{x}_1^{a'}, \mathbf{x}_2^{a'}, \cdots, \mathbf{x}_{K-1}^{a'}) = \mathbf{X}^f \bar{\mathbf{C}}(\bar{\mathbf{\Gamma}}+\mathbf{I})^{-1/2}, \qquad (3)$$

where $\bar{\mathbf{C}}$, a $K\times(K-1)$ matrix, contains the first $K-1$ columns of $\mathbf{C}$ and $\bar{\mathbf{\Gamma}}$ is a $(K-1)\times(K-1)$ diagonal matrix, whose diagonal elements contain the first $K-1$ eigenvalues in $\mathbf{\Gamma}$. Note the sum of columns in $\mathbf{X}^a$ is not zero and we call it one-sided ETKF initial perturbations.

The idea of the spherical simplex centering scheme is to postmultiply $\mathbf{X}^a$ by a $(K-1)\times K$ matrix $\mathbf{U}$ to form K perturbations

$$\mathbf{Y}^a = \mathbf{X}^a\mathbf{U} = (\mathbf{y}_1^{a'}, \mathbf{y}_2^{a'}, \cdots, \mathbf{y}_K^{a'}), \qquad (4)$$

where the matrix $\mathbf{U}$ is selected to ensure that a) the sum of $\mathbf{y}_i^{a'}$, $i=1,\cdots,K$ is zero; b) the analysis error covariance estimated by $\mathbf{X}^a$ is conserved; and c) like $\mathbf{x}_i^{a'}$, the new perturbations $\mathbf{y}_i^{a'}$, $i=1,\cdots,K$, are equally likely. The first requirement is satisfied provided that

$$\mathbf{U}\mathbf{1} = \mathbf{0}, \qquad (5)$$

where $\mathbf{0}$ is a vector with each element equal to zero and $\mathbf{1}$ is a vector with each element equal to one. The second requirement is satisfied provided that

$$\mathbf{U}\mathbf{U}^{\mathrm{T}} = \mathbf{I}, \qquad (6)$$

where $\mathbf{I}$ is the identity matrix. Assuming a multi-dimensional normal distribution, then the third requirement is satisfied by the diagonal elements of $\mathbf{U}^{\mathrm{T}}\mathbf{U}$ must be equal to each other, that is, each column of $\mathbf{U}$ has the same magnitude.

So far we have found two easy solutions to satisfy the three requirements. Because the matrix $\mathbf{U}$ comes from the concepts of spherical simplex sigma point (Julier 1998; Julier and Uhlmann 1996, 2003), we call the ETKF analysis perturbations constructed this way as the spherical simplex ETKF. One of the solutions is a trivial extension of the ETKF. It is easy to verify that $\bar{\mathbf{C}}^{\mathrm{T}}$ in (3) is one solution of $\mathbf{U}$. So the *K* spherical simplex ETKF analysis perturbations are

$$\mathbf{Y}^a = \mathbf{X}^f \bar{\mathbf{C}}(\bar{\mathbf{\Gamma}}+\mathbf{I})^{-1/2}\bar{\mathbf{C}}^{\mathrm{T}}. \qquad (7)$$

For more details of this section please refer to Wang et al. 2003, the complete manuscript.

3 NUMERICAL EXPERIMENT DESIGN

We ran 16-member ensemble plus one control forecast, i.e., $K=16$. We used the same numerical model CCM3 at T42 resolution as in Wang and Bishop (2003). We also used the NCEP/NCAR reanalysis as the control analysis and verification. The time period we consider is the Northern Hemisphere summer in year 2000. The observational network was also assumed to contain only rawinsonde observations. Pseudo-observations were obtained from the reanalysis data by relabeling reanalysis values of wind and temperature at the rawinsonde sites as "observations". The observation error covariance matrix was assumed to be time independent and diagonal. To estimate the error variance of these pseudo-observations, we first calculate 12-h innovation sample variance for wind and temperature at each observation site by averaging all the squared 12-h innovations in the summer of 2000 at each observation site. Then we choose the smallest wind and temperature innovation sample variance of all observation sites as the observation error variance. The inflation factor method is also used (please refer to section 3 in Wang and Bishop 2003 for more details).

4 COMPARISON OF SPHERICAL SIMPLEX AND POSITIVE/NEGATIVE PAIRED ETKF

4.1 Maintenance of Variance along Orthogonal Basis Vectors

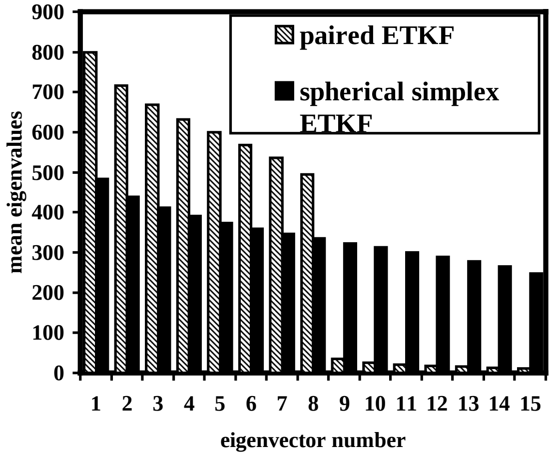

Fig. 1 Seasonally averaged spectra of eigenvalues of 12-h ensemble-estimated forecast error covariance matrices normalized by observation error covariance in observation sites for spherical simplex ETKF and paired ETKF ensembles with 16 perturbed members each.

For an ensemble with 16 perturbed members (i.e. K=16), the short-term error covariance estimates in predicting the true mean and true error covariance have rank 15 for the spherical simplex ETKF scheme, but only 8 for the symmetric positive/negative paired ETKF scheme. This expectation is confirmed by the seasonally averaged eigenvalue spectra for 12-h ensemble-based error covariance matrix in observation space in fig. 1 (see similar plot and definition of the eigenvalue spectra in figure 5 of Wang and Bishop (2003)). While the 12-h ensemble forecast variance for the spherical simplex ETKF ensemble is evenly spread in 15 directions, almost all ensemble variance is maintained in only 8 directions for the symmetric positive/negative paired ETKF ensemble. As a consequence, optimal growth (Wang and Bishop 2003 section 6) within the ensemble perturbation sub-space is larger for the spherical simplex ETKF than for the paired ETKF (not shown).

4.2 Comparison of Initial Ensemble Variance

To compare the performance in estimating the true error variance, we first study how the initial ensemble variance is governed by the geographical variations of observations. Figure. 2 shows the square root of the seasonally and vertically averaged initial wind error variance estimated by the spherical simplex ETKF and the symmetric positive/negative paired ETKF ensembles. For both the spherical simplex ETKF and the paired ETKF ensembles, the initial ensemble variance over the ocean is larger than over the land, which is consistent with the fact that rawinsonde observations are more numerous over the land. The spherical simplex ETKF initial ensemble variance over the Southern Hemisphere (SH) is much larger than over the Northern Hemisphere (NH), which reflects the fact that the rawinsonde is much less distributed in the SH. However, this NH-SH contrast is smaller for the paired ETKF than for the spherical simplex ETKF. This result demonstrates that the spherical simplex ETKF reflects the variation of observation density distribution to a higher degree than the paired ETKF.

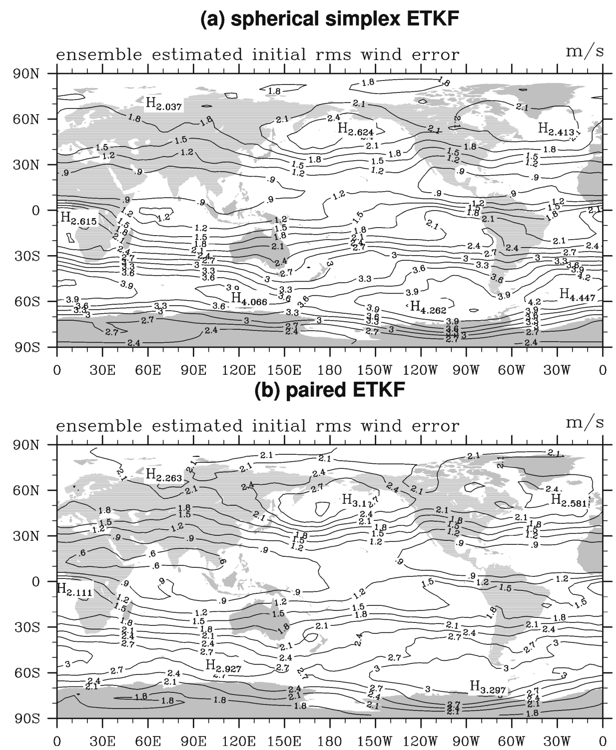

Fig. 2 Square root of seasonally and vertically averaged ensemble wind variance of initial ensemble perturbations for (a) spherical simplex ETKF ensemble and (b) paired ETKF ensemble. Both ensembles have 16 perturbed members plus one control member. The contour interval is 0.3 $m\ s^{-1}$. Label H indicates local maximum.

To better reveal how ensemble spread is governed by the observation density, we plot the rescaling factor that is defined as the ratio of ensemble-estimated initial root mean square (rms) wind error over ensemble estimated 12-h forecast rms wind error. Fig. 3 shows the vertically and seasonally averaged rescaling factor. The effective rescaling factor for the spherical simplex ETKF not only reflects the high concentration of observations over Europe and North America, it is also able to account for the smaller mid-latitude observation concentrations over Southern Hemisphere (SH) continents. In contrast, the rescaling factor of the positive/negative paired ETKF fails to account for these land-based observation concentrations within the Southern Hemisphere.

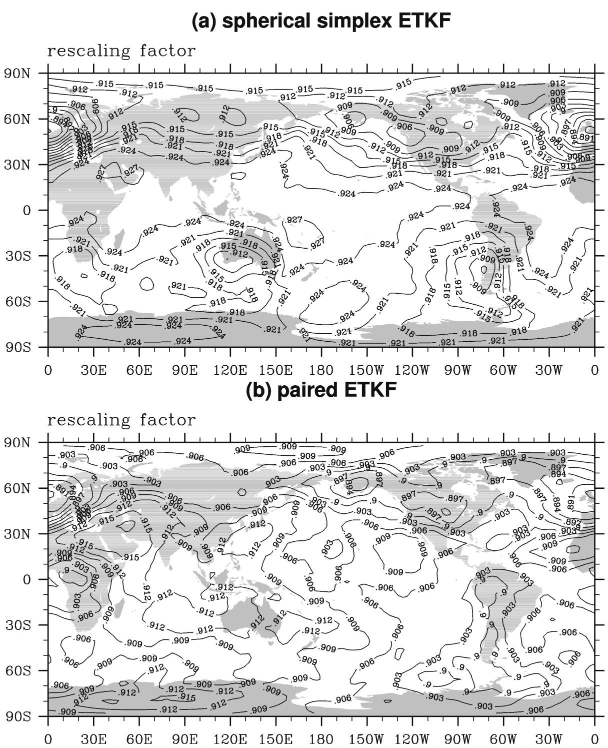

Fig. 3 Seasonally and vertically averaged ratio of ensemble estimated root mean square (rms) initial wind error over ensemble estimated rms 12-h forecast wind error for (a) spherical simplex ETKF and (b) paired ETKF ensembles. Both ensembles have 16 perturbed members and one control member. Contour interval is 0.003.

4.3 Root Mean Square Error of the Ensemble Mean

Fig. 4 shows 200-hPa, 500-hPa and 850-hPa globally averaged ensemble mean forecast error in terms of the approximate energy norm (see definition in equation (26) in Wang and Bishop 2003) for the spherical simplex ETKF, paired ETKF and one-sided ETKF ensembles with 16 perturbed members each. Note for the same ensemble size the one-sided ETKF ensemble has one more subspace rank than the spherical simplex ETKF. The corresponding measurements of control forecast errors are also shown for comparison. The errors are measured against the NCEP/NCAR reanalysis data at every model grid. The ensemble mean of the spherical simplex ETKF is considerably more accurate than the symmetric positive/negative paired ETKF and there is a bit improvement of the spherical simplex ETKF over the one-sided ETKF at all lead times. Although the paired ETKF is centered on the control analysis initially, its ensemble mean is less accurate than that of the one-sided ETKF from 2 to 10-day forecast lead times. These results highlight the importance of resolving as many error directions as possible and indicate that 2nd order accuracy in many directions is better than 3rd order accuracy in a few.

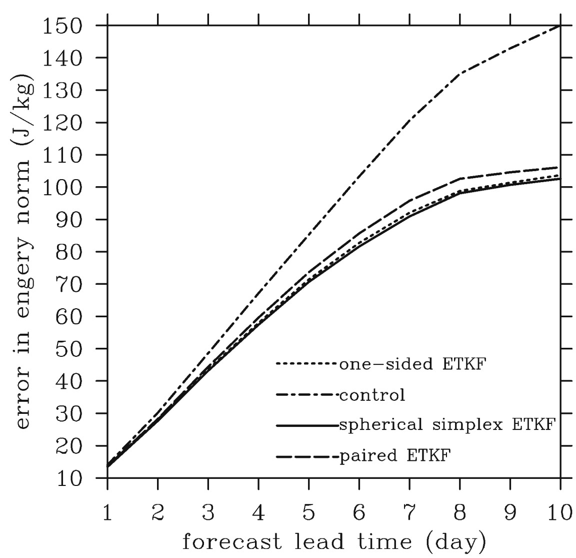

Fig. 4 Globally (all model grids at 200-, 500-, and 850-hPa) and seasonally averaged ensemble mean forecast error in terms of the approximate total energy norm as a function of forecast lead time for the spherical simplex ETKF, paired ETKF and one-sided ETKF ensembles. Each ensemble has 16 perturbed members and one control member. The corresponding measurement of the control forecast error is also shown.

4.4 Comparison of Ensemble Predictions of the Innovation Variance

To compare the skill of the ensemble spread in predicting the forecast error variance, we adopt the methods introduced in section 8 of Wang and Bishop (2003). The results below show that for 1-day and 2-day forecast lead time the skill of the ensemble predictions of the innovation variance from the spherical simplex ETKF significantly outperforms that of the paired ETKF. For longer forecast lead time from 3 to 10 day, their skills become close.

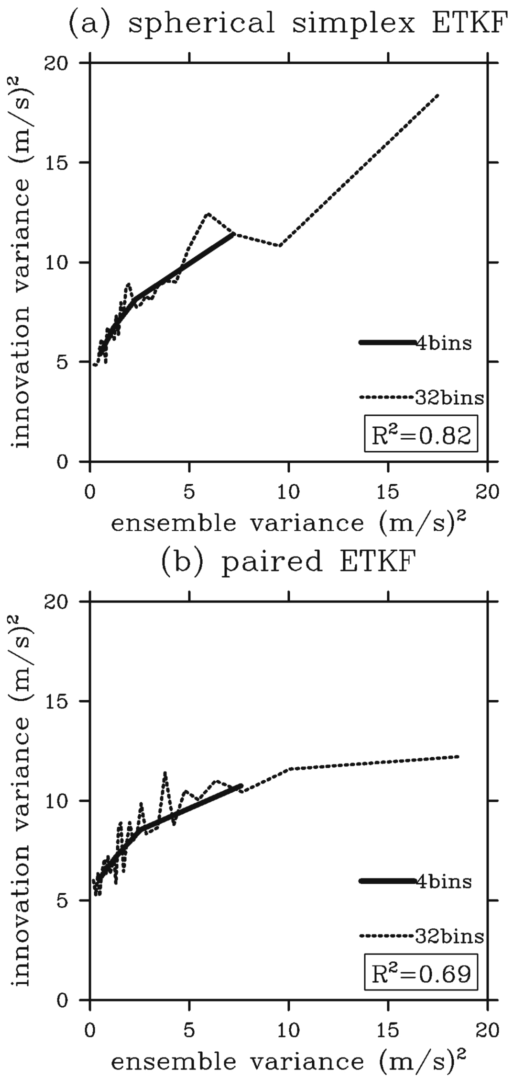

Fig. 5 The relationship between the sample innovation variance and the ensemble variance for the 4-bin case (solid line) and 32-bin case (dashed line) at 1-day forecast lead time. The R-square value on the figure is a measurement on how noisy the dashed curve relative to the solid curve.

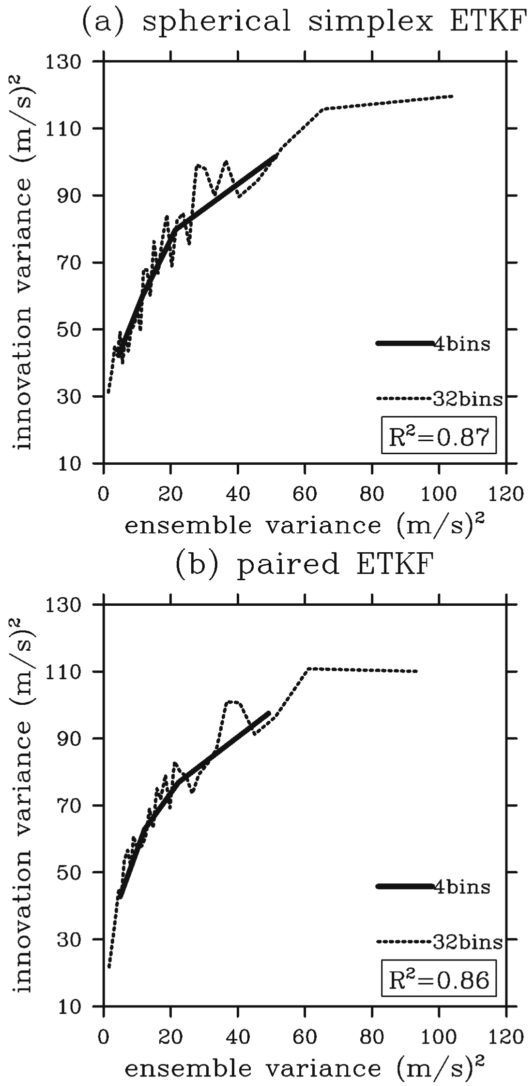

Fig. 6 Same as fig. 5 except for 10-day forecast lead time.

Fig. 5 shows the relationship between the sample innovation variance and the ensemble variance for 500-hPa U at 1-day forecast. This figure is generated by first drawing a scattered plot for which the ordinate and abscissa of each point is respectively given by the squared 500-hPa U wind innovation and 500-hPa U wind ensemble variance at 1-day forecast at one midlatitude observation location. The innovation is defined here as the difference between the verifying analysis and the 1-day ensemble mean forecast at the rawinsonde observation sites. Points collected correspond to all midlatitude stations and all 1-day 500-hPa U forecasts throughout the NH summer in year 2000. To begin, we divide the points into four equally populated bins, arranged in order of increasing ensemble variance. Then we average the squared innovation and ensemble variance in each bin, respectively. Connecting the averaged points then yields a curve describing the relationship between the sample innovation variance and the ensemble variance. The results corresponding to the 4-bin and 32-bin cases for 1-day forecast lead time are shown in figure 5. First, note that the range of innovation variance resolved by the spherical simplex ETKF ensemble variance is much larger than that of the paired ETKF. A statistical test based on halving the data size was used to confirm this result. Second, as the sample size in each bin is decreased (e.g., from 4-bin case to 32-bin case), the relationship between sample innovation variance and the ensemble variance for 1-day forecasts becomes noisier for the paired ETKF than for the spherical simplex ETKF. The noisiness is measured by the R-square value (Ott 1993) for the dashed curve relative to the solid curve. Less noisiness corresponds to large R-square value. A *t* test (Ott 1993) is used to confirm that the R-square value of the spherical simplex ETKF is significantly larger than that of the paired ETKF. According to the analysis in section 8 of Wang and Bishop (2003), these results show that for 1-day (true for 2-day as well, not shown) forecast, the ensemble spread of the spherical simplex ETKF is more accurate in predicting the forecast error variance than that of the paired ETKF. Our result also shows that for longer forecast lead time from 3 to 10 day, the skills of the two centering schemes in predicting the innovation variance become statistically indistinguishable. Figure 6 which is the result for 10-day forecast lead time illustrates this point.

5 SUMMARY

In this paper, we tested the performance of two ensemble centering schemes for the ETKF ensemble generation scheme. One was the common symmetric positive/negative paired centering and the other was the spherical simplex centering. In the spherical simplex scheme, one more perturbation was added to one-sided ETKF initial perturbations such that a). the sum of the new set of initial perturbations equaled zero, b). the covariance of the new perturbations was equal to the analysis error covariance matrix obtained from the one-sided ETKF initial perturbations, and c). all the new initial perturbations were equally likely.

The spherical simplex ETKF ensemble mean was found to be more accurate than the mean of the positive/negative paired ETKF ensemble. For an ensemble of *K* perturbed members, the spherical simplex ETKF maintained comparable amounts of variance in $K-1$ orthogonal and uncorrelated directions as compared to only *K*/2 directions for the paired ETKF. The initial ensemble variance from the spherical simplex ETKF better reflected the geographical variations of the observations than the paired ETKF. The spherical simplex ETKF can discriminate a significantly larger range of sample innovation variance than the paired ETKF for 1 day and 2 day forecast lead times. Because the spherical simplex ETKF initial perturbations are generated by simply postmultiplying the one-sided ETKF initial perturbations by a $(K-1)\times K$ matrix (section 2) where *K* is the number of perturbed members, the computational expense of generating the spherical simplex ETKF ensemble is as small as that of generating the symmetric positive/negative paired ETKF ensemble.

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