1. INTRODUCTION

A practical way for providing probabilistic forecasts is through ensemble forecasting. In ensemble forecasting, the probability distribution function (PDF) at the initial time is represented by a finite sample of possible initial conditions. A nonlinear model integration is performed on each of these states. If 1) the deficiencies of the numerical model are negligible, and 2) the sample of initial states provides a realistic estimate of the probability distribution of the control analysis errors, then the ensemble forecast produces a realistic distribution of forecast states and thus the relative frequency of forecast model outcomes can be used to generate calibrated probabilistic forecasts.

So far, most operational centers focus on the generation of initial perturbations with the assumption that the forecast model is perfect. The best method for generating initial perturbations is still in debate. Of all ensemble generation schemes, the breeding method (Toth and Kalnay 1993, 1997) developed and applied by the National Center for Environmental Prediction (NCEP) is the most computationally inexpensive. The fundamental hypothesis of this method is that analysis errors are filtered forecast errors. In the simplest form of the breeding method, forecast perturbations are transformed into analysis perturbations by multiplying each of the forecast ensemble perturbations by a constant factor whose magnitude is less than one. Thus, the effect of variations in the distribution of observation sites on the analysis errors is neglected. Furthermore, directions corresponding to slowly growing modes may be completely filtered out from the ensemble perturbation subspace, which implies that there is a danger of breeding modes becoming parallel to each other.

The ensemble transform Kalman Filter (ETKF) theory of Bishop et al. (2001) suggests an alternative method of recycling or breeding perturbations to that suggested in Toth and Kalnay (1993, 1997). The ETKF ensemble generation scheme produces perturbations by solving the equation relating analysis error covariance to forecast error covariance for an optimal data assimilation scheme within the vector subspace of forecast error covariance for an optimal data assimilation scheme. The ensemble transform Kalman Filter (ETKF) theory was optimal. For an optimal data assimilation scheme, the ensemble forecast produces a realistic probability distribution of the control analysis errors, but also provides a framework for generating ensemble perturbations.

Different from the breeding method that transforms forecast perturbations into analysis perturbations by multiplying each of the forecast ensemble perturbations by a constant factor whose magnitude is less than one, the ETKF method transforms forecast perturbations into analysis perturbations by a transformation matrix $T$, that is,

$$Z^a = Z^f T,$$  \hspace{1cm} (1)

where forecast perturbations are listed as columns in the matrix $Z^f$ and analysis perturbations are listed as columns in the matrix $Z^a$. The transformation matrix $T$ is chosen in order to ensure that the covariance matrix associated with the transformed perturbations $Z^a$ would be precisely equal to the true analysis error covariance matrix $P^a$ if the covariance matrix of the raw forecast perturbations were equal to the true forecast error covariance matrix $P^f$ and the data assimilation scheme were optimal. For an optimal data assimilation scheme,

$$P^a = P^f - P^f H (H P^f H^T + R)^{-1} H P^f,$$  \hspace{1cm} (2)

where the matrix $H$ is the observation operator that maps model variables to observed variables and the matrix $R$ is the observation error covariance matrix.

As shown in Bishop et al. (2001), if

$$P^f = Z^f (Z^f)^T,$$  \hspace{1cm} (3)

then equation (2) is satisfied by letting

$$P^a = Z^a (Z^a)^T,$$  \hspace{1cm} (4)

provided

$$T = C (\Gamma + I)^{-1/2},$$  \hspace{1cm} (5)

where columns of the matrix $C$ contain the eigenvectors, and the elements of the diagonal matrix $\Gamma$ contain the corresponding eigenvalues of $(Z^f)^T H R^{-1} H Z^f$. Note that since

$$T^T (Z^a)^T H R^{-1} H Z^a T = \Gamma (\Gamma + I)^{-1},$$  \hspace{1cm} (6)

the analysis perturbations are orthogonal in observation space under a Euclidean norm normalized by the observation error covariance.

The matrix $(Z^a)^T H R^{-1} H Z^a$ is KxK where K is the number of ensemble perturbations. Consequently, the main computations required for ETKF ensemble generation are the KxK inner products in observation space required to form the elements of $(Z^a)^T H R^{-1} H Z^a$. 

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together with the eigenvector decomposition of $(Z^*)^T H R^T H Z^*$. The number of operations required for these computations is much less than that required for the generation of singular vector (SV) perturbations (Buizza and Palmer, 1995; Molteni et al., 1996) or system simulation ensembles (Houtekamer et al., 1996). In the example to be presented here, ETKF ensemble generation was only slightly more expensive than breeding.

Since ETKF generation rotates and rescales perturbations according to equation (2), it is the distribution and quality of observations that controls perturbation amplitude. Furthermore, consistent with the filtering properties of an optimal data assimilation scheme, ensemble variance is reduced in directions corresponding to large forecast error variance more than it is in directions corresponding to small forecast error variance. Thus, one would expect ETKF generated ensemble perturbations to retain a wide range of uncorrelated amplifying directions.

3. NUMERICAL EXPERIMENT

To test our expectations about the qualitative differences between the two techniques, we ran 16-member (one control forecast and 15 perturbed forecasts) T42 NCAR Community Climate Model (CCM3) ensembles starting from the NCEP/NCAR reanalysis data for both the ETKF and breeding methods for the boreal (NH) summer in 2000. For the ETKF ensemble generation scheme, it is assumed that the observational network consisted solely of rawinsondes released every 12 hours at the sites shown in Fig. 1. For both methods, the maximal likelihood parameter estimation theory (Dee, 1995) is used to ensure that the 12-hour forecast ensemble variance is consistent with control forecast error variance at rawinsonde observation sites.

4. COMPARISON OF THE BREEDING AND THE ETKF METHODS

4.1 Initial Perturbations

Fig. 2 compares square roots of the seasonal mean vertically averaged ensemble wind variance at the analysis time for the breeding method (Fig. 2a) and the ETKF method (Fig. 2b). First, initial perturbation amplitude in the observation scarce Southern Hemisphere is much larger for the ETKF method than it is for the breeding method. Second, despite the high concentration of rawinsondes over the Eurasian continent, the initial breeding perturbation amplitude is locally maximized in this region. In contrast, the initial ETKF perturbation amplitude is quite small in this region. The manner in which this 16-member ETKF generation method has allowed ensemble spread to be governed by observational density is better seen by plotting maps of the ratio of vertically and seasonally averaged analysis root mean square (rms) wind error over vertically and seasonally averaged forecast rms wind error. Such maps give a representation of the geographical distribution of the factor that rescales 12-hour forecast ensemble spread into 0-hour ensemble spread. Figs 3a and 3b display this ratio for the 8-member and 16-member ETKF ensembles, respectively. Fig 3b shows that the effective rescaling factor for the 16-member ETKF ensemble not only reflects the high concentrations of observations over Europe and North America, it also crudely accounts for the smaller mid-latitude concentrations over South Africa, Australia and South America. The superiority of the 16-member results over the 8-member results leads us to suspect that the sensitivity of ETKF ensemble rescaling factors to variations in observational density would be further improved by moving to a 32-member ensemble.
Fig. 3 The ratio of vertically and seasonally averaged analysis rms wind error over vertically and seasonally averaged 12-hour forecast rms wind error. Values in the shaded area are equal or less than 0.92 that is the median of the contour levels with interval 0.01 for both (a) and (b).

Fig. 4 Boreal summertime mean of eigenvalues. White and black columns pertain to the 16-member breeding and the 16-member ETKF ensembles respectively.

4.2 Ensemble Subspace

Fig. 4 compares the seasonal mean spectrums of eigenvalues of the ensemble based 12-hour forecast error covariance matrices for the 16-member breeding ensemble and the 16-member ETKF ensemble. The spectrum of ETKF eigenvalues is much flatter than that of the breeding eigenvalues. In other words, while there are large amounts of ensemble forecast variance present in all 15 uncorrelated orthogonal directions of the ETKF ensemble, nearly all of the breeding ensemble forecast variance is contained in a single direction. Furthermore, for the breeding ensemble there is nearly zero variance in the three uncorrelated orthogonal directions corresponding to the smallest three eigenvalues. Although such severe rank reduction would be inhibited by the masks used in the form of the breeding method used operationally at NCEP, it is still a cause for concern.

4.3 Ensemble Skill

A quick evaluation on the quality of the breeding and ETKF ensembles for the 8-member ensembles is performed by comparing the error variance of the ensemble mean and the error correlation between ensemble members. Table 1 shows the average correlation and the ensemble mean error variance of 1 to 5 day forecasts of 250 hPa temperatures at global rawindsone sites for both the breeding and the ETKF ensemble. It turns out that throughout 1 to 5 day forecasts the breeding ensemble is more correlated than the ETKF ensemble and the ensemble mean of the breeding ensemble is less accurate than that of the ETKF ensemble. Presumably, the relatively large error correlation found for both techniques in 5-day forecasts is due to model error.

Because the ensemble mean does not represent an optimal combination of either breeding or ETKF ensemble members, a comparison on the skill of optimal combinations of ensemble forecasts is needed. The optimal combinations are obtained from the covariances of the errors in each of the ensemble forecasts via a straightforward application of the estimation theory by Cohn (1997). Table 1 shows that the optimal combination of the breeding ensemble is less accurate than that of the ETKF ensemble.

5. SUMMARY AND DISCUSSION

The ETKF ensemble generation scheme transforms forecast perturbations into analysis perturbations by solving the equation relating the forecast and analysis error covariances of an optimal data assimilation scheme within the ensemble perturbation subspace. Consequently, analysis perturbation magnitudes reflect the density and accuracy of observations and analysis perturbations are orthogonal in observation space. In addition, the directions corresponding to large forecast error variance in observation space are attenuated more than the directions corresponding to small forecast error variance. Each ETKF analysis perturbation represents a linear combination of forecast perturbations. Thus, assuming forecast perturbations are balanced, ETKF
analysis perturbations are also balanced provided forecast perturbation amplitude is small enough to justify a linearization of the balance equation.

The computational expense of the ETKF technique is very small compared to that of the singular vector technique and the system simulation approach. In the examples considered here, the computational expense of the ETKF technique was within 5% of the breeding technique.

The breeding ensemble generation technique is similar in spirit to the ETKF technique in that it views analysis perturbations as filtered forecast perturbations. Here we have compared the performance of a simple form of the breeding technique in which each ensemble perturbation is rescaled by a constant factor that ensures that, on average, forecast perturbation magnitude is consistent with the forecast error of the control forecast against the ETKF generation technique. We illustrated that while breeding mode analysis perturbation amplitude is modulated solely by dynamics, ETKF analysis perturbation amplitude is modulated by dynamics and the geographic distribution of observations. We showed that while the error variance of a 16-member T42 CCM3 breeding ensemble was concentrated in a single direction, the ETKF 16-member ensemble error variance was evenly spread amongst 15 independent, orthogonal, and uncorrelated directions.

Forecast errors of 250 hPa temperature were found to be more highly correlated in the breeding mode ensemble than in the ETKF ensemble. The ETKF ensemble mean was found to be more accurate than the breeding ensemble mean. Having pointed out that the mean is a non-optimal combination of ensemble forecasts when the control forecast is more accurate than the ensemble members, we also showed that the optimal combination of ETKF ensemble members for the season was superior to the corresponding optimal combination of the breeding ensemble members.

Future work will compare the merits of obtaining better observational network resolution by increasing ensemble size against the merits of obtaining better observational network resolution by letting the transformation matrix $T$ be a slowly varying function of latitude. This slowly varying function would be achieved by only letting observations within a certain distance of a grid point influence the value of $T$ at that grid point. We are also interested in testing the ability of the ETKF technique to forecast the forecast error variance.

<table>
<thead>
<tr>
<th>day</th>
<th>(a) ensemble error correlation</th>
<th>(b) ensemble mean error variance</th>
<th>(c) optimal combination error variance</th>
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</thead>
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<tr>
<td>1</td>
<td>ETKF 0.5142 BRED 0.8327</td>
<td>ETKF 2.602 BRED 2.992</td>
<td>ETKF 2.571 BRED 2.601</td>
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<tr>
<td>2</td>
<td>ETKF 0.6572 BRED 0.8680</td>
<td>ETKF 3.410 BRED 3.808</td>
<td>ETKF 3.387 BRED 3.513</td>
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<tr>
<td>3</td>
<td>ETKF 0.7131 BRED 0.8762</td>
<td>ETKF 4.030 BRED 4.506</td>
<td>ETKF 4.007 BRED 4.266</td>
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<tr>
<td>4</td>
<td>ETKF 0.7358 BRED 0.8784</td>
<td>ETKF 4.690 BRED 5.095</td>
<td>ETKF 4.663 BRED 4.933</td>
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<tr>
<td>5</td>
<td>ETKF 0.7478 BRED 0.8757</td>
<td>ETKF 4.690 BRED 5.095</td>
<td>ETKF 4.663 BRED 4.933</td>
</tr>
</tbody>
</table>

Table 1. A comparison of the ensemble forecast skill between the 8-member breeding and ETKF ensembles for the global 250hPa temperature in boreal summer of 2000. (a) averaged correlation of the ensemble forecast errors. (b) averaged error variance of the ensemble mean forecasts. (c) averaged error variance of the optimal combination of the ensemble forecasts.

6. REFERENCES


