Evolution of Forecast Error Covariances in 4D-Var and ETKF methods

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Introduction

Estimates of forecast error covariances are at the heart of any data assimilation system and yet the way they are modelled in any operational assimilation scheme is limited by the compromises made for practical implementation and the available knowledge of the statistical properties of the forecast error. In most operational assimilation schemes the forecast error covariance is assumed stationary, homogeneous and isotropic to overcome the difficulty of estimating the full covariance matrix. These assumptions fail to characterise the 'true' forecast error covariance.

The purpose of this study is to estimate the 'true' forecast error covariance for use in variational data assimilation and to disentangle the contribution of the initial condition error from the model error. This is achieved by examining three approaches which differ according to their strategy and underlying assumptions to generate the data samples required to define the forecast error covariance. The paper also focuses on the evolution of these error covariances over 24 hours.

The ensemble-based covariances are estimated by propagating the full non-linear model in time starting from initial conditions generated by an ETKF. The error covariance evolution implied by 4D-Var is estimated by drawing a random sample of initial conditions from a Gaussian distribution with the standard deviations given by the background error covariance matrix and then evolving the sample foward in time using linearised dynamics. Finally the growth of the standard deviation of the deterministic forecast error averaged over a large numer of cases is evaluated as benchmark of the climatological error. Although the three methods rely on different assumptions and are limited by their own approximations, by using these three techniques in conjunction, we may improve our knowledge of the forecast error covariance and produce a better estimate of the 'true' forecast error covariance.

The paper is organised as follows: the first section discusses the different assumptions and limitations of the three methods. The second section describes the relevant approaches to diagnose the forecast error statistics. The third section presents the results of the forecast error estimations and their evolution over a 24 hour period. The final section provides a summary of this study.

1 Formulation of forecast error covariances

1.1 Forecast Error Covariances in 4D-Var

In this study we will focus on the Met Office 4D-Var in its incremental form which become operational at the Met Office in October 2004. 4D-Var minimises a four dimensional cost function in which a forecast model is used as a constraint in the assimilation process to propagate the initial model state to the times of the observations. The minimisation is performed at a lower resolution than the main forecast, with simpler physics and using a cost function evaluated by integrating a linearised forecast model rather than the full non linear model [1, 2]. Within each assimilation window the model is assumed perfect, all errors in the problem are assumed unbiased and uncorrelated, so that they can be represented by a zero mean Gaussian distributions.

The hypothesis of perfect model is not tenable because the model resolution is a limitation in resolving the exact solution of the governing equations. The perfect model assumption though reduces the complexity and expenses of 4D-Var and makes it achievable operationally. The assumption of unbiased errors is deficient in practise because there often are significant biases in the background fields and in the observations, whereas the hypothesis of uncorrelated errors is usually valid since error sources in the background and in the observations are supposed to be completely independent (except for error sources between observations). The assumption of linearity is strong. Incremental 4D-Var relies on the linearization of weakly non-linear operators, at the expense of optimality of the analysis.

In current operational meteorological models, the dimension of the model state N is of the order of 10^7 per analysis, therefore the background error covariance matrix contains $10^7 \times 10^7$ distinct coefficients, which are estimated statistically. Its full structure cannot be determined or even stored with modern computers, and, even if this was possible, there is no enough statistical information to determine all its elements.

It is usual to denote background (i.e. short-term forecast) error covariances by $\mathbf{P}$:

$$\mathbf{P} =< (\mathbf{x}^b - \mathbf{x}^t)(\mathbf{x}^b - \mathbf{x}^t)^T > . \tag{1}$$

Here the angled brackets denote the expected value of forecast errors $\mathbf{x}^b - \mathbf{x}^t$, where $\mathbf{x}^t$ is the 'true' state of the atmosphere which is unknown, and $\mathbf{x}^b$ is the background state. This $\mathbf{P}$ matrix is unknown and is prohibitive to calculate. For this reason the background error covariance used in 4D-Var, denoted by $\mathbf{B}$, is a simplification of $\mathbf{P}$. The possible ways to estimate $\mathbf{B}$ without the knowledge of the true state $\mathbf{x}^t$ will be discussed in Section 2.

In practical implementations of 4D-Var, no cycling of covariances takes place and at each analysis cycle the forecast error covariance at the beginning of the assimilation period is replaced by the static background error covariance $\mathbf{B}$. However the covariance matrix $\mathbf{B}$ is implicitly propagated in time according to the linearised dynamics to generate flow dependency at later times within the assimilation window. Under the approximations of linear error growth and small model error, the short-forecast error covariance within 4D-Var is given approximately by $\mathbf{P} = \mathbf{MBM}^T$, where $\mathbf{M}$ is the linearised forecast model integrated over the period of the assimilation.

1.2 Forecast Error Covariances in the ETKF

It is well known that for the linear case and a perfect model, 4D-Var analysis at the end of the assimilation period is equivalent to the Kalman filter analysis over the same interval, given the same inputs. However, the Kalman filter is impractical for large dimensional systems, since it requires to handle $N \times N$ covariance matrices and it has to calculate N integrations of the linear forecast model $\mathbf{M}$ to propagate the covariance matrix of the analysis error.

For large systems approximate Kalman filters (or reduced-rank methods) have been developed in order to restrict the covariance equations to a small subspace. Ensemble Kalman Filters (EnKF) are an example of reduced-rank Kalman filters where the background covariance matrix ($\mathbf{P}_k^b$) at time k is constructed as sample covariances:

$$\mathbf{P}_k^b \approx \frac{1}{K}\sum_{i=1}^{K}\left(\mathbf{x}_k^{b(i)} - \overline{\mathbf{x}_k^b}\right)\left(\mathbf{x}_k^{b(i)} - \overline{\mathbf{x}_k^b}\right)^T \tag{2}$$

where the index i refers to the ensemble member, K is the number of ensemble members and $\overline{\mathbf{x}_k^b} = \frac{1}{K}\sum_{i=1}^{K}\mathbf{x}_k^{b(i)}$

is the ensemble mean forecast. In this way the sample covariance matrix represents an estimate of the true covariance matrix restricted to the subspace of the ensemble. If K is small (e.g. $K \sim 100$), the analysis error covariance may be propagated using only K model integrations and $\mathbf{P}^b_{k+1}$ may be projected onto a new subspace to generate an approximate covariance matrix to be used in the next analysis cycle. The EnKF method still assumes that all the errors are Gaussian.

The EnKF is an approximation of the full Kalman filter and it is not optimal, because the analysis are restricted onto the space spanned by the ensemble members and the approximated $\mathbf{P}^b_k$ presents spurious long-range correlations. However, ensemble methods are attractive because they do not require the tangent linear or adjoint operators. In the EnKF method the covariances are estimated using a limited size sample equal to the number of the ensemble members and by propagating model states with a fully non linear model.

MOGREPS (Met Office Global and Regional Ensemble Prediction System) is an Ensemble Transform Kalman Filter (ETKF) where the ensemble of analysis is calculated by transforming the background states of the previous cycle [3]. In the ETKF method the analysis perturbations for each cycle are a linear combination of the forecast perturbations. The ETKF transformation matrix rotates and rescales the forecast perturbations according to the geographical location and accuracy of the observations [3, 4, 5, 6]. In MOGREPS the analysis perturbations are then added to the Met Office 4D-Var analysis to provide the initial conditions for the ensemble members forecasts. To compensate the lack of the representation of the background error covariance outside the subspace defined by the ensemble forecasts, MOGREPS uses a variable inflation factor to ensure that the forecast ensemble spread matches the error of the ensemble-mean forecast at some lead time and at the radiosonde observation locations [3, 7]. In addition to the representation of model error resulting from the inflation factor, a model error term is also used in MOGREPS. This is represented by using stochastic-physics schemes, which aim to describe the effects of physical processes occurring at scales not resolved by the model and to account for model uncertainties associated with empirical model parameters. The use of stochastic physics together with the ETKF implies adding model perturbations to the initial condition perturbations so that the effect due to the initial conditions or to model errors is more difficult to untangle.

1.3 Forecast error covariance in Verification

The verification of operational forecasts usually relies on the assumption that the unknown 'true' state of the atmosphere is well represented by the observations or by the verifying analysis at the forecast lead time. The verification against the observations does not provide a global information on the forecast error statistics, whereas when using the analysis as verifying state of the atmosphere climatological estimate of the forecast error statistics can be easily calculated.

The mean error (m.e.) is given by the time average over a month of differences between forecast and analysis verified at the same time:

$$\text{m.e.} = < \mathbf{x}^f(t) - \mathbf{x}^a(t) >_t \tag{3}$$

where $\mathbf{x}^f(t)$ is the high resolution deterministic forecast at time t, $\mathbf{x}^a(t)$ is the verifying analysis valid at time t and $<>$ denotes the time average. The root mean square error (r.m.s.e.) then is:

$$\text{r.m.s.e.} = \sqrt{< (\mathbf{x}^f(t) - \mathbf{x}^a(t))^2 >_t}. \tag{4}$$

The main limitation of this approach is given by the sample size and by the fact that the statistical sample characterises a climatological forecast error in which each realisation represents a single weather case condition.

2 Estimation of Forecast Error Covariances

As already mentioned the estimation of the covariance matrix of the background error is difficult. This is because the ‘true’ background state to measure the errors against is unknown and a surrogate state must be used instead, the size of the **B** matrix is unfeasibly large and there is no enough accurate data to calibrate statistics.

In general, a way to estimate error statistics is to assume that they are uniform over a domain and stationary over a period of time. In this way one can make empirical statistics by taking a number of error realisations (i.e. climatological errors). Additional approximations used in modelling the background error covariance, such as isotropy, homogeneity and closeness to balance, partially compensate the missing information needed to estimate such a large covariance matrix [8, 9].

Useful information on the error statistics can be gathered from diagnostics of an existing data assimilation system using the innovation method (described in [10]) and the NMC method (described in Section 2.1). Flow-dependency of forecast error covariances can be estimated directly from a Kalman filter. Climatological forecast error statistics can be also generated by an ensemble method (described in Section 2.2).

2.1 NMC method

The most common choice in operational centres for a surrogate of the forecast error is to use differences between forecasts of different lengths that are valid at the same time. This method is known as the NMC method [11]:

$$\mathbf{B} \approx \frac{1}{2} < \left(\mathbf{x}^{t_2} - \mathbf{x}^{t_1}\right) \left(\mathbf{x}^{t_2} - \mathbf{x}^{t_1}\right)^T > \tag{5}$$

where $\mathbf{x}^{t_2}$ and $\mathbf{x}^{t_1}$ are pairs of forecasts valid at the same time and the angle brackets represent the averaging over a period of many assimilation cycles. Typically pairs of forecasts differ by 24 hours in order to avoid diurnal cycle errors interpreted as background errors, as in the following:

$$\begin{aligned} \mathbf{x}^{t_2} &= \mathscr{M}_{0\to t_2}\mathbf{x}^a(t=0) \\ \mathbf{x}^{t_1} &= \mathscr{M}_{24\to t_1}\mathbf{x}^a(t=24) \end{aligned}$$

where $\mathscr{M}$ is the full non-linear forecast model evolving the analysis $\mathbf{x}^a$ at the specified times. Since the background is usually a 6 h forecast, the Met Office operationally uses $t_2 = 30$ h and $t_1 = 6$ h forecast differences as proxy for forecast errors.

The method assumes that the statistical structure of forecast errors do not vary much over a period of t_2 hours, and that the forecast errors at times t_2 and t_1 are uncorrelated and have a similar statistical structure to that of background errors.

2.2 Ensemble method

Another method to produce a surrogate of the forecast errors is the ensemble method [12]. Here we describe only the ensemble method used in this study for generating proxy for background errors. This method uses the MOGREPS ensemble in which the initial condition perturbations are produced by the ETKF and model error is added to each ensemble member through a stochastic physics approach.

For the estimation of the climatological **B** matrix the averaging is made over many assimilation cycles:

$$\mathbf{B} \approx \left\langle < \left(\mathbf{x}^b - \mathbf{x}^*\right) \left(\mathbf{x}^b - \mathbf{x}^*\right)^T >_{\text{ens}} \right\rangle_{\text{time}} \tag{6}$$

where the angled brackets $<>_{\text{ens}}$ and $<>_{\text{time}}$ represent the averaging over K ensemble members at a particular time and over many assimilation cycles respectively. Here $\mathbf{x}^*$ represents the 'truth', which can be chosen to be the ensemble mean or the verifying analysis for that particular assimilation cycle considered. By calculating differences of ensemble members from the verifying analysis, the covariance statistics take into account the model error as well as the growth in spread.

As the NMC method, the ensemble method produces global statistics of the model variables at all levels but with a much larger sample size over a month of assimilation cycles. Moreover, the ensemble method computes the statistics from forecasts of the same length as the background (i.e. 6 h).

3 Results and discussion

In standard 4D-Var there is effectively no cycling of errors as the forecast error covariance matrix at each analysis time is replaced by the static **B** covariance matrix and implicitly evolved within the analysis window. On the other hand, the Kalman filter methods explicitly evolves the covariance matrix but in order to keep the error variances realistic a model error term is required. Here we compare the results of the evolution of the background error using the MOGREPS ensemble and the implicit evolution of 4D-Var when the initial conditions are represented by a random sample of the Met Office's operational background error covariance matrix.

The MOGREPS system consists of both global and regional forecasts. Here in this study we consider only the global prediction system. MOGREPS global ensemble consist of 24 members and it is run twice a day starting at 00 UTC and 12 UTC for 72 hours.

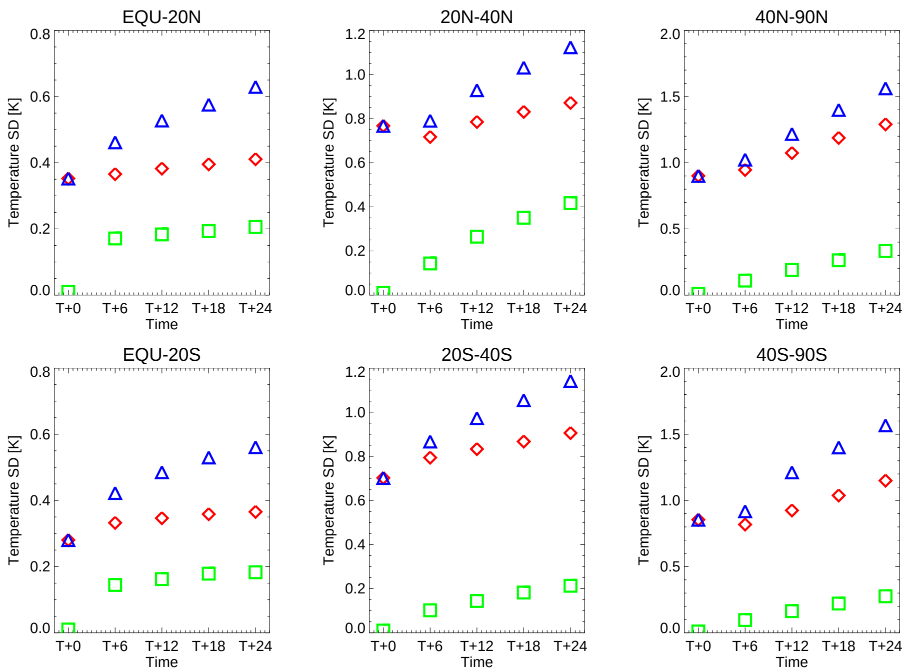

Figure 1: Background error evolution for temperature at 500 hPa. The red diamonds represent the ensemble spread growth and the blue triangles represent the evolution of the ensemble spread and the model error. The green squares represent the evolution of the model perturbations generated by MOGREPS stochastic physics.

Figure 1 shows the evolution of temperature background error at 500 hPa over 24 hours calculated using the ensemble method. The error evolution is split in six latitude bands: EQU – 20N, 20N – 40N, 40N – 90N in the top three panels and EQU – 20S, 20S – 40S, 40S – 90S in the bottom three panels. In Fig. 1 and all following figures, the red diamonds represent the ensemble spread growth (or initial condition perturbation growth, used in the followings as synonymous) when the error is measured against the ensemble mean and the blue triangles represent the evolution of the ensemble spread and the model error i.e. when the error is measured against the verifying analysis. As the time evolves the background error grows faster when the model error is included (i.e. blue triangles). In the extra-tropics the ensemble spread and the model error evolutions are similar for the first 6 hours and then they tend to separate, while in the equatorial regions the separation occurs earlier. In particular, in the region 40N – 90N the ensemble spread matches quite well the model error evolution. This may be explained by the fact that MOGREPS uses a variable inflation factor to ensure that the ensemble spread matches the ensemble mean error at T+12 h and at the radiosondes locations, more dense in the Northern Hemisphere. This implies not only that MOGREPS is correctly tuned in the Northern Hemisphere extra-tropics for temperature at 500 hPa, but also that the ensemble spread evolution contains some elements of model error coming from this tuning.

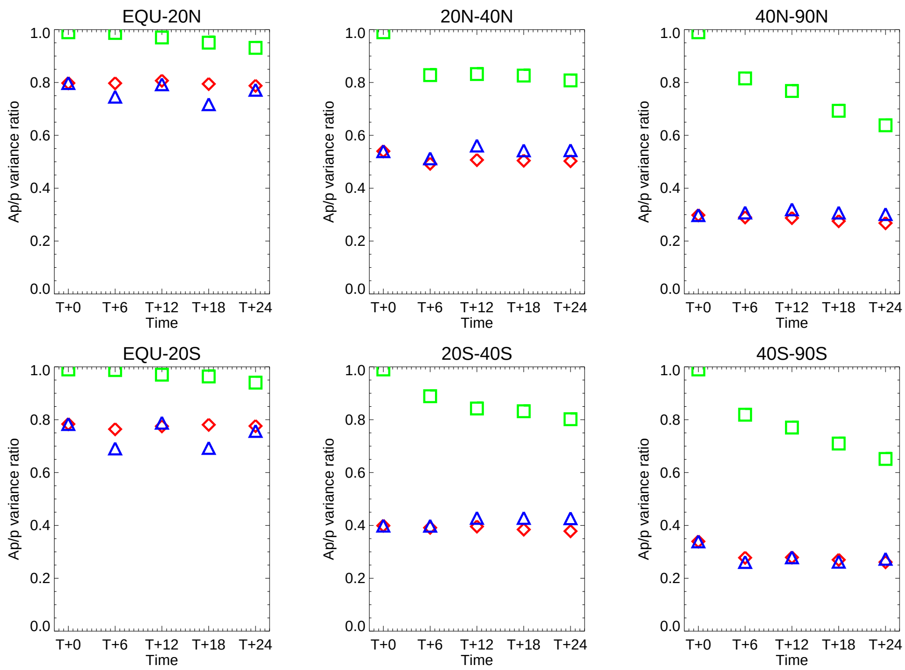

Figure 2: As Fig. 1 but for the ratio of unbalanced pressure over total pressure at 500 hPa.

In both cases (i.e. red diamonds and blue triangles), the initial condition perturbations include also the stochastic physics perturbations. In order to estimate the contribution of the stochastic physics to the initial condition error and its evolution in time, the initial condition perturbations coming from the ETKF have been removed and only the model perturbations have been used as perturbations. This error evolution is represented in Fig. 1 by the green squares for temperature at 500 hPa. The contribution from the stochastic physics scheme is small, of the order of 10% in the tropics and extra-tropics and slightly higher in the equatorial regions.

Figure 2 shows instead the evolution of the ratio of unbalanced pressure over total pressure errors over 24 hours at 500 hPa. This ratio represents the remaining unbalanced component of the flow in the system after imposing the geostrophic balance relationship. In the extra-tropical regions the stochastic physics perturbations mainly introduce imbalance in initial conditions of pressure at 500 hPa (i.e. green squares). On the other hand when the stochastic physics perturbations are added to the ETKF perturbations (i.e. red diamonds or blue triangles) the initial conditions are still in balance and stay in balance over the 24 hour period.

Now we want to compare the error growth estimated using the ensemble method to the 4D-Var error growth. The evolution of the forecast error covariance is implicit in the 4D-Var system. The randomisation method, described in [13] and [14], provides a diagnosis of the background errors at the beginning of the assimilation period, when $\mathbf{B}$ is of the form $\mathbf{B} = \mathbf{U}\mathbf{U}^T$. If ξ_l is a set of L random vectors in control variable space drawn from a Gaussian distribution with zero mean and unit variance, then applying $\mathbf{U}$ to this set of random vectors gives a distribution with covariance matrix $\mathsf{B} \sim \frac{1}{L}\sum_{l=1}^{L}(\mathbf{U}\xi_l)(\mathbf{U}\xi_l)^T$. These background errors at the beginning of the assimilation window are then evolved with the linearised model dynamics for 24 hours to simulate the flow dependency of 4D-Var within the assimilation window. The 4D-Var error evolution is shown in Fig. 3 by the green stars and compared with the MOGREPS spread evolution (red diamonds) for temperature at 500 hPa. In the extra-tropics 4D-Var initial condition error does not grow as much as the ensemble spread. In principle both sets of data should not include any systematic components, although the tuning effect of MOGREPS introduces a systematic adjustment to the ensemble spread.

At first the lack of growth in 4D-Var was surprising because we expected the linearised model dynamics to exaggerate the growth compared to the non-linear full dynamics used in the evolution of the ensemble initial condition. One explanation may be that the randomisation method selects a random sample of initial condition perturbations which do not project onto rapidly growing structures while MOGREPS selects fast growing modes that quickly develop in forecast errors. In addition the covariance model imposes homogeneity and isotropy to reduce the amount of information needed to estimate the background error covariance in 4D-Var which may explain the lack of rapidly amplifying structures expected when using a linear model.

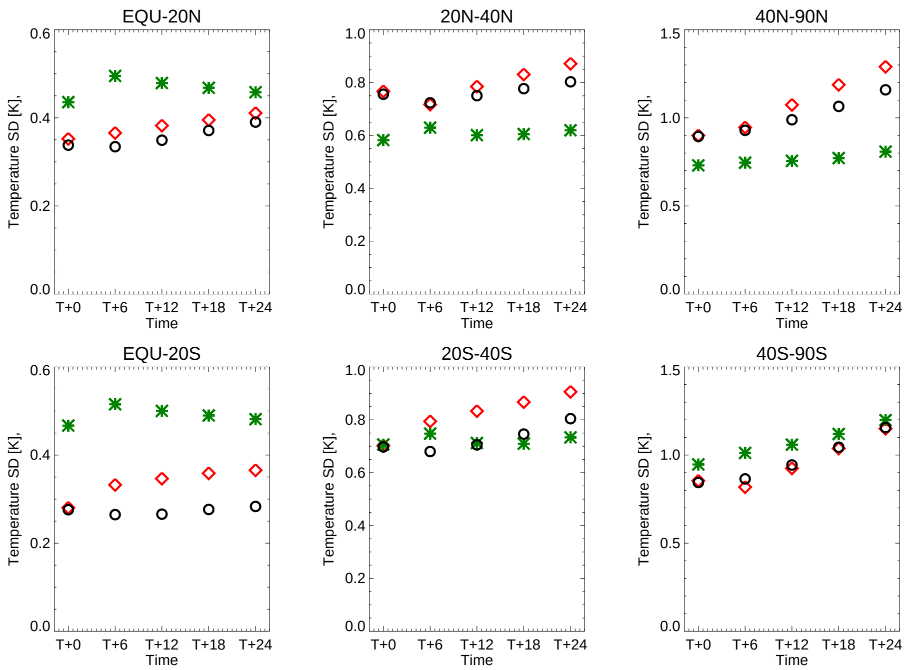

Figure 3: Background error evolution for temperature at 500 hPa. The red diamonds represent the ensemble spread growth, the green stars the 4D-Var evolution and the black circles represent the linear evolution of the MOGREPS perturbations.

In order to make a clean comparison, we decided to evolve MOGREPS initial condition perturbations with the same linearised model dynamics used by 4D-Var. Figure 3 shows such comparison for temperature at 500 hPa, where the linear evolution of MOGREPS perturbations is represented by the black circles. First, we expect the linear (black circles) and non-linear (red diamonds) evolution of the ensemble spread to have similar growth. This is the case for the Northern Hemisphere regions and for 40S – 90S. Differences in EQU – 20S and 20S – 40S regions may be explained mainly by two different effects: the resolution of the full non-linear model is higher than the linearised model's resolution (120 km in mid-latitudes compared to the 40 km) and most of the physics of the non-linear model is omitted [1] which leads to enhance the physics effect in these two regions (i.e. Southern hemisphere summer cases) where convection is more active.

When we compare the linear evolution of MOGREPS perturbations (black circles) with 4D-Var (green stars) in Figure 3, we notice that they show similar initial condition error growth in the Southern Hemisphere extra-tropics, while in the Northern Hemisphere extra-tropics MOGREPS shows more growth. This may be explained again by the tuning of the ensemble spread, since the cycling inflation factor is calibrated better in the Northern Hemisphere. In the equatorial regions the evolution of the error is similar although there is an offset between MOGREPS and 4D-Var perturbations at T+0 which persists during the 24 hours error evolution.

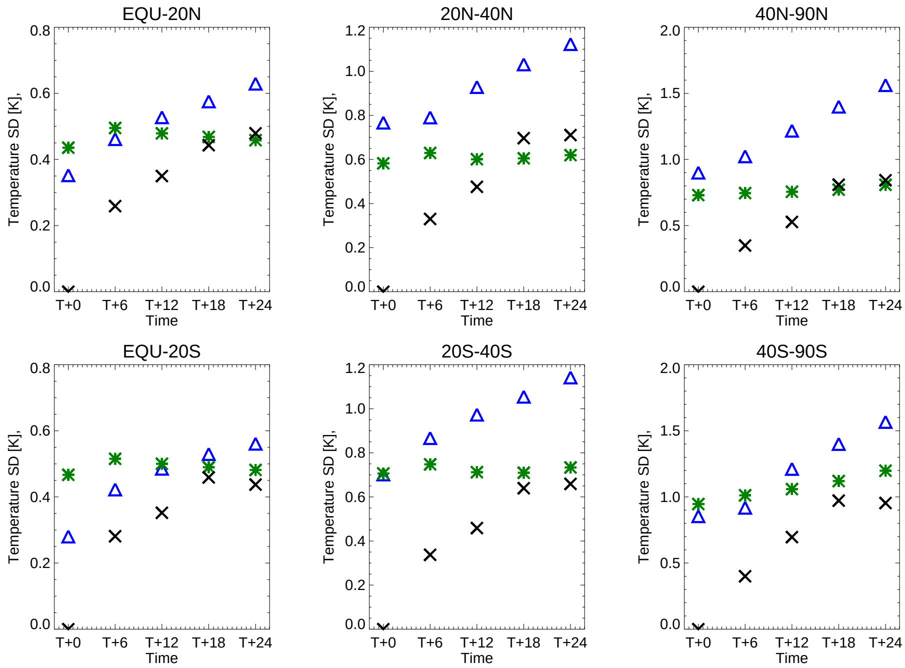

Figure 4: Background error evolution for temperature at 500 hPa. The blue triangles represent the evolution of the ensemble spread and the model error, the green stars the 4D-Var evolution and the black crosses the climatological verification error.

Finally in Fig. 4 we compare MOGREPS and 4D-Var error growth with the climatological error. The verification error represent the error of the deterministic forecast measured against the verifying analysis averaged over one month of cases. It includes the model error due to model deficiencies in the model integration. Therefore, the verification error represents our benchmark for forecast error. In Fig. 4 we compare first the verification error (black crosses) with MOGREPS error evolution when the error is measured against the verifying analysis (blue triangles), which contains also the model error contribution. For all six latitude bands, the verification error is smaller and generally shows an offset compared to MOGREPS model error evolution. This offset is clearly due to the lack of ensemble spread in the verification error since it represents a single estimate of the forecast error averaged over one month. The implicit error growth in 4D-Var (green stars) is different from both MOGREPS model error evolution and verification error. In particular, 4D-Var is in general smaller than the MOGREPS model error and larger than the verification error. In principle it should not include any systematic errors, but the background error covariance used here has been calculated using the NMC method which contradicts 4D-Var assumption of zero mean initial condition error because it includes a model error through the different time lengths of the model integration.

4 Summary

The forecast error covariance matrix is a key element in any data assimilation systems. A number of compromises and assumptions are required in order to face the computational challenge of estimating the full covariance matrix used for NWP systems. The lack of knowledge of the statistical properties of the forecast error and the enormous size of its error covariance require either important simplifications in the covariance modelling or to derive the error statistics from surrogate quantities.

In this paper we have presented three methods with the aim of improving our knowledge of the 'true' forecast error covariance matrix and understanding whether the initial condition error and model error contribution are separable. Even though all these three methods have their own limitations and approximations, all methods contribute to a better undertanding of the forecast error covariance matrix. The ensemble-based covariance methods represent better the 'true' forecast error covariance when all different error contributions are included. In the case of the MOGREPS ensemble since the ETKF perturbations are very well balanced, the forecast error may not properly represent the 6 h background error which may not be balanced. It also remains a puzzle how well 4D-Var performs despite the lack of growth of its forecast error covariances. In both cases though it is not possible to distinguish model error from initial condition error growth.

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