Modelling of forecast errors in geophysical fluid flows

R. N. Bannister^{1, *, †}, D. Katz², M. J. P. Cullen³, A. S. Lawless² and N. K. Nichols²

¹Department of Meteorology, University of Reading, P.O. Box 243, Reading RG6 6BB, U.K. ²Department of Mathematics, University of Reading, P.O. Box 220, Reading RG6 6AX, U.K. ³Met Office, Fitzrov Road, Exeter EX1 3PB, U.K.

SUMMARY

A method is sought to decompose errors in numerical forecasts of the atmosphere into components that are uncorrelated. This can simplify the representation of the probability density function of forecast errors so that it can be used in data assimilation. A new method based on potential vorticity (PV) is used to partition errors into balanced and unbalanced variables that are thought to be mutually uncorrelated. The effectiveness of the PV method is compared with a simpler method. A toy model and an operational forecasting model are used to show that the PV-based variables are usually less correlated than those of the simpler approach. Copyright © 2007 John Wiley & Sons, Ltd.

Received 25 April 2007; Revised 17 August 2007; Accepted 17 August 2007

KEY WORDS: data assimilation; forecast error covariances; potential vorticity; meterology; unified model; shallow water equations

1. FORECAST ERRORS IN DATA ASSIMILATION

Forecasts from numerical weather prediction (NWP) models have improved greatly since they were first produced routinely 50 years ago, partly due to their improved initial conditions, \mathbf{x}_{ic} . Data assimilation (DA) estimates \mathbf{x}_{ic} by making a short forecast, \mathbf{x}_f of the current weather, which is in error. This is then adjusted to fit observations where the adjusted state, $\mathbf{x}_{ic} = \mathbf{x}_f + \mathbf{x}'$, has a smaller error than \mathbf{x}_f . The adjustment, \mathbf{x}' , is restricted by the prescribed forecast error probability density function (PDF). Good forecasts depend on accurate characterization of the PDF, and we report on a practical approach that may allow this to be represented compactly.

^{*}Correspondence to: R. N. Bannister, Data Assimilation Research Centre, Department of Meteorology, University of Reading, P.O. Box 243, Reading RG6 6BB, U.K.

[†]E-mail: r.n.bannister@reading.ac.uk

Contract/grant sponsor: Natural Environment Research Council Contract/grant sponsor: Met Office

Let forecast error be defined as ε' in $\mathbf{x}_f = \mathbf{x} + \varepsilon'$, where \mathbf{x} is the 'true state'. The PDF of ε' , $P_f(\varepsilon')$, specifies the probability that the forecast has error ε' . A Gaussian with mean zero is the usual choice for $P_f(\varepsilon')$, which is described by the forecast error covariance matrix, \mathbf{B}_{ε}

$$P_{\rm f}(\boldsymbol{\varepsilon}') \sim \exp{-\frac{1}{2}\boldsymbol{\varepsilon}'^{\rm T} \mathbf{B}_{\varepsilon}^{-1} \boldsymbol{\varepsilon}'} \tag{1}$$

The PDF, $P_f(\varepsilon')$, is combined with observational information to give $P_{\text{comb}}(\mathbf{x})$, which is used in the DA problem. By (1) and Bayes' rule [1], $P_{\text{comb}}(\mathbf{x})$ is

$$P_{\text{comb}}(\mathbf{x}) \sim \exp{-\frac{1}{2}(\mathbf{x} - \mathbf{x}_{\text{f}})^{\text{T}} \mathbf{B}_{\varepsilon}^{-1}(\mathbf{x} - \mathbf{x}_{\text{f}})} \times P_{\text{ob}}(\mathbf{y}|\mathbf{x})$$
(2)

In (2), $P_{ob}(\mathbf{y}|\mathbf{x})$ is the PDF that the observations (in **y**) are true given **x**. In variational DA, **x** is found by maximizing $P_{comb}(\mathbf{x})$ (actually by minimizing $-\ln P_{comb}(\mathbf{x})$).

We use potential vorticity (PV) to seek a new representation of \mathbf{B}_{ε} that may be described well using a block diagonal matrix. In Section 2 we describe the toy and NWP models (and their balance relationships) that we use, in Section 3 we introduce PV and in Section 4 we propose how PV may help to achieve our goal. This is demonstrated in Section 5 and summarized in Section 6.

2. THE NUMERICAL MODELS AND THEIR BALANCE RELATIONS

2.1. One-dimensional shallow water equation model of the atmosphere

The shallow water equations (SWEs) for a rotating fluid describe air motion in a layer. We consider the SWEs for a quasi 1-D atmosphere. The SWEs are a standard model of the atmosphere which, when posed in 1-D, gives the simplest non-trivial model that can be used to study forecast errors. Katz *et al.* [2] introduce the SWEs for *u* and *v* (fluid velocities in the *x* and *y*-directions), and *h* (depth of the layer), but we show equivalent equations for ψ (streamfunction), χ (velocity potential) and *h*

$$\frac{\partial}{\partial t} \left(\frac{\partial^2 \psi}{\partial x^2} \right) + u \frac{\partial}{\partial x} \left(\frac{\partial^2 \psi}{\partial x^2} \right) + \left(\frac{\partial^2 \psi}{\partial x^2} + f \right) \left(\frac{\partial^2 \chi}{\partial x^2} \right) = 0$$

$$\frac{\partial}{\partial t} \left(\frac{\partial^2 \chi}{\partial x^2} \right) + u \frac{\partial}{\partial x} \left(\frac{\partial^2 \chi}{\partial x^2} \right) + \left(\frac{\partial^2 \chi}{\partial x^2} \right)^2 - f \left(\frac{\partial^2 \psi}{\partial x^2} \right) + g \frac{\partial^2 (H+h)}{\partial x^2} = 0, \quad \frac{\partial h}{\partial t} + \frac{\partial hu}{\partial x} = 0$$
(3)

Here H(x) is the orographic height, f is the (constant) Coriolis parameter and g is the gravitational acceleration. The grid has 500 points; hence, the state vector $\mathbf{x} = (\psi, \chi, h)^{\mathrm{T}}$ comprises 1500 elements and \mathbf{B}_{ε} has 2.25×10^{6} matrix elements.

Fields ψ and *h* are related approximately by the linear balance equation (LBE) $f \partial \psi / \partial x = g \partial (H+h) / \partial x$, which holds well at mid-latitudes. Linearizing about $\bar{\psi}$ and \bar{h} , such that $\psi = \bar{\psi} + \psi'$ and $h = \bar{h} + h'$, gives the LBE in perturbation form [2] $f \partial \psi' / \partial x = g \partial h' / \partial x$. This is an exact relationship between the parts, $\psi'_{\rm h}$ and $h'_{\rm h}$ that are 'in balance' with each other (the remaining

Copyright © 2007 John Wiley & Sons, Ltd.

parts, ψ'_u and h'_u —and χ' —are said to be 'unbalanced' [3,4]). We write this (i) after integrating (and assuming zero integration constants) and (ii) after differentiating:

$$f\psi'_{\rm b} - gh'_{\rm b} = 0, \quad f\left(\frac{\partial^2\psi'_{\rm b}}{\partial x^2}\right) - g\left(\frac{\partial^2h'_{\rm b}}{\partial x^2}\right) = 0$$
 (4)

2.2. The Meteorological Office's Unified Model

The Unified Model (UM) [5] used by the Met Office for NWP is based on the primitive equations and can be specified in terms of ψ , χ and p plus other variables. In the UM, f is variable and pressure, p, is analogous to h in the SWEs. The model domain used has $216 \times 162 \times 50$ points. Considering only ψ , χ and p, the state vector $\mathbf{x} = (\psi, \chi, p)^{T}$ has 5.2×10^{6} elements and \mathbf{B}_{ε} has 2.8×10^{13} elements. For the UM system, a LBE is applicable for perturbations between the balanced wind and balanced pressure

$$\nabla_{\mathbf{h}} \cdot (f \bar{\rho} \nabla_{\mathbf{h}} \psi_{\mathbf{b}}') - \nabla_{\mathbf{h}}^2 p_{\mathbf{b}}' = 0$$
⁽⁵⁾

where ∇_h is the 2-D differential operator at constant height.

For the UM, \mathbf{B}_{ε} is too large to use, but the problem can be reduced with a transformation to variables whose errors are decoupled. Our strategy is to find variables whose errors are expected to be uncorrelated, using properties of PV to do this for the SWEs and UM.

3. THE PV

A useful quantity called PV [6] can be defined for the SWE and UM systems. For the SWEs the PV is $q_{\text{SWE}} = h^{-1}(f + \partial^2 \psi / \partial x^2)$. A linearized perturbation form, q'_{SWE} , is used here [2]

$$q'_{\rm SWE} = \frac{1}{\bar{h}} \left(\frac{\partial^2 \psi'}{\partial x^2} - \bar{q} h' \right) \tag{6}$$

where an overbar is a reference state quantity. For the UM, the appropriate PV is called Ertel PV, q_{Ertel} , and is approximated as follows [7] (factors $\bar{\alpha}$, $\bar{\beta}$, $\bar{\gamma}$ and $\bar{\eta}$ are specified in [7]):

$$q'_{\text{Ertel}} = \bar{\alpha} \nabla_{\rm h}^2 \psi' + \bar{\beta} p' + \bar{\gamma} \frac{\partial p'}{\partial z} + \bar{\eta} \frac{\partial^2 p'}{\partial z^2}$$
(7)

PV is useful for two reasons. Firstly, it can be inverted: given PV, suitable boundary conditions and a balance relation, the 'balanced' component of the flow—i.e. (ψ'_b, χ'_b, h'_b) in the case of the SWEs and (ψ'_b, χ'_b, p'_b) in the case of the UM—can be diagnosed $(\chi'_b = 0 \text{ as } \chi' \text{ does not contribute to PV})$. Secondly, according to linear theory, the balanced flow associated with PV evolves independently from (and hence uncorrelated with) the unbalanced flow (see, e.g. [8]). The PV-based balanced and unbalanced variables are introduced in Section 4.

It is common to assume that ψ'_b is equal to the total perturbation ψ' , thus avoiding the need to use PV. We call this the 'balanced vorticity approximation' (BVA). The BVA-based variables, which are currently used to represent \mathbf{B}_{ε} at the Met Office, are introduced in Section 4.2. The BVA is good (i.e. $\psi' \approx \psi'_b$ is true) when the horizontal scale of the flow is much less than the Rossby radius, $L_R = \sqrt{gh}/f$ [3, 4]. This holds in the tropics where f is small.

Copyright © 2007 John Wiley & Sons, Ltd.

R. N. BANNISTER ET AL.

4. NEW VARIABLES BASED ON PV

Diagnosis of the balanced flow is useful because this component is believed to evolve in a way that is largely decoupled from the unbalanced flow. Let v'_{PV} be a representation of forecast error, ϵ' in terms of the following balanced/unbalanced variables.

- For the balanced field we choose $\psi'_{\rm b}$, which is described entirely in terms of PV.
- For the first unbalanced field we choose χ' , which has no associated PV.
- For the second unbalanced field we choose unbalanced height, h'_{u} , for the SWEs and unbalanced pressure, p'_{u} , for the UM, which also have no associated PV.

Illustrating for the SWE, $\mathbf{v}'_{PV} = (\psi'_b, \chi', h'_u)^T$, which has error covariance matrix:

$$\mathbf{B}_{\mathrm{PV}} = \begin{pmatrix} \mathbf{B}_{\psi'_{b}\psi'_{b}} & \mathbf{B}_{\psi'_{b}\chi'} & \mathbf{B}_{\psi'_{b}h'_{u}} \\ \mathbf{B}_{\psi'_{b}\chi'}^{\mathrm{T}} & \mathbf{B}_{\chi'\chi'} & \mathbf{B}_{\chi'h'_{u}} \\ \mathbf{B}_{\psi'_{b}h'_{u}}^{\mathrm{T}} & \mathbf{B}_{\chi'h'_{u}}^{\mathrm{T}} & \mathbf{B}_{h'_{u}h'_{u}} \end{pmatrix}$$
(8)

If variables in \mathbf{v}'_{PV} are uncorrelated, then this matrix will simplify: $\mathbf{B}_{\psi'_b\chi'}=0$, $\mathbf{B}_{\psi'_bh'_u}=0$ and $\mathbf{B}_{\chi'h'_u}=0$. Then \mathbf{v}'_{PV} can be used in a transformed form of (1) with $\mathbf{B}_{\varepsilon} \rightarrow \mathbf{B}_{PV}$ [3]. The hypothesis that \mathbf{B}_{PV} is block diagonal is expected to hold in a linear system, but neither the SWE nor UM is linear and the UM includes parametrizations for radiative, moist and sub-grid-scale processes that lead to correlations. The hypothesis that the PV error covariance matrix is block diagonal for these systems is tested in Section 5.

4.1. Transformations using PV

The PV and the LBE are used to compute \mathbf{v}'_{PV} . The method is shown for the SWEs, but the principle extends to the UM. A forecast error from (3) $(\psi', \chi', h')^T$ is to be determined in terms of $(\psi'_b, \chi', h'_u)^T$. The first variable, ψ'_b , is described by PV. This means that (6) can be written as

$$q'_{\rm SWE} = \frac{1}{\bar{h}} \left(\frac{\partial^2 \psi'}{\partial x^2} - \bar{q}h' \right) = \frac{1}{\bar{h}} \left(\frac{\partial^2 \psi'_{\rm b}}{\partial x^2} - \bar{q}h'_{\rm b} \right) = \frac{1}{\bar{h}} \left(\frac{\partial^2 \psi'_{\rm b}}{\partial x^2} - \frac{\bar{q}f}{g} \psi'_{\rm b} \right)$$
(9)

using the LBE (4). The solution, ψ'_{b} , is unique as long as $\bar{q}f$ is positive, which is expected to hold. This equation can be solved by Fourier transforms, but the analogous 3-D equation for the UM is more difficult to solve (we use the Generalized Conjugate Residual solver).

The second variable, χ' , is already a prognostic variable in (3) and hence needs no processing. For the third variable, h'_{u} , substitute in (4) ψ' and h'. This will not give zero since only the balanced parts will satisfy (4). The residual is called the 'linear imbalance' or 'anti-PV', ζ'_{a} :

$$\zeta_a' = f \frac{\partial^2 \psi'}{\partial x^2} - g \frac{\partial^2 h'}{\partial x^2} = f \frac{\partial^2 \psi_u'}{\partial x^2} - g \frac{\partial^2 h_u'}{\partial x^2}$$
(10)

The full perturbations have balanced and unbalanced parts, $\psi' = \psi'_b + \psi'_u$ and $h' = h'_b + h'_u$, and since the balanced parts satisfy (4), ζ'_a is equivalently expressed with the unbalanced parts only, as has

Copyright © 2007 John Wiley & Sons, Ltd.

been done in (10). The unbalanced fields have zero PV; hence, from (6), $\partial^2 \psi'_u / \partial x^2 = \bar{q} h'_u$. The term $\partial^2 \psi'_u / \partial x^2$ can then be eliminated from (10), giving

$$f\frac{\partial^2 \psi'}{\partial x^2} - g\frac{\partial^2 h'}{\partial x^2} = f\bar{q}h'_{\rm u} - g\frac{\partial^2 h'_{\rm u}}{\partial x^2}$$
(11)

The solution, h'_{u} , is unique as long as $\bar{q}f$ is positive. This is similar to (9) and is solved in a similar way. An analogous 3-D equation for p'_{u} exists for the UM system.

4.2. Transformations using the BVA

Equations (9) and (11) may be avoided using the BVA where, unlike in Section 4.1, the streamfunction is taken to be completely balanced. Then the following set of fields are used to describe the forecast errors.

- The 'balanced' variable is ψ' —this is already a forecast perturbation field.
- The first unbalanced variable is χ' —this is also already a forecast perturbation field.
- The second unbalanced variable is called $h'_{\rm r}$. It is the unbalanced height under the BVA and is found from the residual of the LBE (4), $h'_{\rm r} = h' h'_{\rm b} = h' (f/g)\psi'$.

For the BVA, $\mathbf{v}'_{\text{BVA}} = (\psi', \chi', h'_r)^T$ (with $h'_r \rightarrow p'_r$ for the UM system). The assumption that ψ' , rather than ψ'_b , describes the 'balance' is often unrealistic. In Section 5 the correlations between elements of \mathbf{v}'_{BVA} are compared with those between \mathbf{v}'_{PV} . This is important for the UM because the BVA is used to represent forecast errors in the Met Office's operational DA system [9].

5. NUMERICAL EXPERIMENTS

A sample of errors, $\{\epsilon'\}$, are transformed into $\{v'_{PV}\}$ and $\{v'_{BVA}\}$ for the SWE and UM systems and used to compute correlations between the variables.

5.1. Correlations for the one-dimensional SWE model

We integrate the SWEs under different flow regimes, described here by two parameters. The Burger number, Bu, is the ratio L_R/L , where L is the horizontal lengthscale. At large Bu (small horizontal scales), the BVA is expected to be good [3, 4]; hence, we expect similar results from \mathbf{v}'_{PV} and \mathbf{v}'_{BVA} . The Rossby number is Ro = U/fL, where U is the characteristic wind. Small Ro indicates that mass and wind are related well by (4). As Ro increases, the LBE becomes more approximate and nonlinearity becomes more important.

Figure 1 shows correlations $cor(\psi'_b, h'_u)$ for $\mathbf{v'_{PV}}$ and $cor(\psi', h'_r)$ for $\mathbf{v'_{BVA}}$ as a function of *Ro* for high and low *Bu*. For high *Bu* (Figure 1(a)), where the BVA is good, the correlations are small for $\mathbf{v'_{PV}}$ (solid line) and $\mathbf{v'_{BVA}}$ (dashed line). The correlations for PV variables are higher than for BVA variables at the larger *Ro*, probably due to the increasing nonlinearity (the PV transformations rely on linearity), but are still small. For small *Bu* (Figure 1(b)), where the BVA is not good, the PV variables show consistently small correlations at all *Ro* shown, unlike the BVA variables. Correlations involving χ' (not shown) are small for all cases. The results show that it is reasonable to ignore correlations between PV variables but not between BVA variables in the 1-D SWE system. Further results of these experiments are shown in [2].



Figure 1. Correlations between balanced wind and unbalanced height errors for the SWEs.



Figure 2. Zonal mean correlations between balanced and unbalanced variables for the UM, calculated from a set of six states. Dotted lines depict negative values and the zero line is thick. Contours are for every 0.1.

5.2. Correlations for the unified model

In the UM it is not possible to control Bu or Ro. Plotted in Figure 2 are $cor(\psi'_b, p'_u)$ in \mathbf{v}'_{PV} and $cor(\psi', p'_r)$ in \mathbf{v}'_{BVA} . Correlations for PV variables (Figure 2(a)) are large. These are due to inherent properties of the UM and/or inaccuracies in the solution of the UM's equivalent of (9) and (11) (the 3-D solver's residuals ranged 3–25% of the prescribed PV or anti-PV). Disentangling these is further work. Correlations for PV variables though are smaller than BVA variables (Figure 2(b)) on average by 0.1, demonstrating an advantage of using PV.

Copyright © 2007 John Wiley & Sons, Ltd.

MODELLING OF FORECAST ERRORS

6. SUMMARY

PV can help define new variables that partition forecast errors into balanced and unbalanced parts. This is useful if the forecast error covariance matrix in terms of these variables is to be well represented by a block diagonal matrix. The off-diagonal correlations are examined in a simple 1-D and a full 3-D atmospheric model. The correlations between the balanced and unbalanced variables (PV variables) are compared with those between quasi-balanced and unbalanced variables which inappropriately treat the rotational wind as balanced (BVA variables). In the SWEs the PV variables, unlike the BVA variables, have small correlations for all flow regimes tested. In the UM correlations are large but are smaller for the PV variables than for the BVA variables. This shows some benefit in using PV variables for DA. In solving UM analogues of (9) and (11), we found large residuals using the 3-D solver, leaving scope to improve the UM results with another solver.

ACKNOWLEDGEMENT

This work has been assisted financially by Natural Environment Research Council (NERC) and the Met Office. During the course of this work the authors acknowledge useful comments with Andrew Lorenc, David Pearson, Ian Roulstone and Marek Wlasak, and are grateful for the suggestions made by the two reviewers.

REFERENCES

- 1. Lorenc AC. Analysis methods for NWP. The Quarterly Journal of the Royal Meteorological Society 1986; 112(474):1177–1194.
- Katz D, Lawless AS, Nichols NK, Cullen MJP, Bannister RN. A comparison of potential vorticity-based and vorticity-based control variables. *Numerical Analysis Report 8/2006*, Department of Mathematics, University of Reading, 2006; 1–34. Available at www.maths.rdg.ac.uk/research/publications/Na_reports.asp.
- 3. Cullen MJP. Four dimensional variational data assimilation: a new formulation of the background-error covariance matrix based on a potential vorticity representation. *The Quarterly Journal of the Royal Meteorological Society* 2003; **129**(593):2777–2796.
- 4. Wlasak MA, Nichols NK, Roulstone I. Use of potential vorticity for incremental data assimilation. *The Quarterly Journal of the Royal Meteorological Society* 2006; **132**(621):2867–2886.
- Davies T, Cullen MJP, Malcolm AJ, Mawson MH, Staniforth A, White AA, Wood N. A new dynamical core for the Met Office's global and regional modelling of the atmosphere. *The Quarterly Journal of the Royal Meteorological Society* 2005; **131**(608):1759–1782.
- 6. Gill AE. Atmosphere–Ocean Dynamics, vol. 30. Academic Press: San Diego, 1982.
- 7. Bannister RN, Cullen MJP. The implementation of a PV-based leading control variable in variational data assimilation. Part 1: transforms. *DARC Technical Report*, vol. 6, 2003; 1–29. Available at darc.nerc.ac.uk/int_rpt_6/PVcv.pdf.
- 8. Daley R. Atmospheric Data Analysis. Cambridge University Press: Cambridge, MA, 1991.
- 9. Ingleby NB. The statistical structure of forecast errors and its representation in the Met Office global 3-dimensional variational data assimilation system. *The Quarterly Journal of the Royal Meteorological Society* 2001; **127**(571): 209–231.