Numerical Weather Prediction

On the choice of control fields in Var

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A. Lorenc, I. Roulstone and A. White

email: nwp_publications@metoffice.com

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Abstract

The control fields that are the subject of this report are the fields whose forecast errors are (ideally) uncorrelated and which result from the parameter transform in Var as described by Lorenc *et al.* (2000). We are not primarily concerned with the decomposition of the control fields into vertical and horizontal modes (the amplitudes of which are the final control variables in Var). Streamfunction, velocity potential, unbalanced pressure and relative humidity are currently the chosen control fields. We discuss the issues involved in the choice of control fields, considering both geostrophically balanced and unbalanced elements and exploring a number of possible choices for each. The report consists of a main text that is almost an equation-free zone and four Appendices giving mathematical detail relevant to the curent scheme and to possible modifications of it.

Contents

1. Motivation & introduction

Variational analysis seeks an initial model state that represents the best compromise between observations and a "background" state obtained from a previous forecast model run.

Our variational analysis scheme involves three basic transformations (and their inverses). The first transformation is from the model's fields to new *control fields* whose forecast errors are only weakly correlated with one another. Ideally, errors in these control fields would be totally uncorrelated with one another, and the forecast error covariance matrix $\mathbf{B}$ (see Appendix 1) would be of block diagonal form. In practice, this ideal is unattainable but we strive to approach it; we seek fields whose errors are very weakly correlated, and then (as a working hypothesis) disregard the residual correlations between errors in different fields. The transform from model fields to nearly uncorrelated fields (in the sense of errors) is known locally as the *parameter transform* or the T_p *transform.* The inverse transform is called the U_p *transform.* The design of the parameter transform is the main subject of this paper.

The second and third transforms are carried out to improve the conditioning of the linear equations for the best-compromise initial state, and involve the introduction of horizontal and vertical *modes.* These transformations are an essential ingredient of our variational analysis scheme, but they are not the main subject of this paper. Bannister (2000) gives a clear overview of both the parameter and mode transforms.

Whether or not it is of block diagonal form, the error covariance matrix $\mathbf{B}$ is symmetric and positive definite. As outlined in Appendix 1, this endows the eigenvectors of $\mathbf{B}$ with various useful properties. For example, a procedure may be constructed to find the square root $\mathbf{U}$ of $\mathbf{B}$ (such that $\mathbf{B} = \mathbf{U}\mathbf{U}^T$); also, an ordered expansion in terms of the eigenvectors of $\mathbf{B}$ maximises the variance explained in a truncated series. For discussion of the parameter transform we need apply only a simple analogue of the latter result. We may seek to reduce correlations between different control fields (and thus to promote block-diagonal structure of $\mathbf{B}$) by choosing later control fields to be residuals: we subtract from that field (e.g. pressure) all that can be predicted from a knowledge of the leading control field. [Here we assume that fields which are themselves uncorrelated also have uncorrelated errors.]

2. Balanced control fields

We assume that the most important (largest) modes of background error are hydrostatically and (in some sense) geostrophically balanced; we want our first control field to describe these modes. So we need to choose a scalar field which defines, and is defined by, the balanced flow. Three candidates have been suggested: rotational wind (i.e. streamfunction), mass field (i.e. pressure) and PV (or a PV-related streamfunction). In choosing between them, the following criteria must be considered:

1. How well does the field characterise the balanced flow?
2. How accurately can we "invert" the field to calculate a well-balanced PF state?
3. How well can we model the 3-dimensional error structure using our horizontal and vertical transforms?
4. How difficult are the transforms to code, remembering we want the control-field-to-model-field transform (U), its adjoint (U_hat), and its inverse (T)?

How well do the candidate fields characterise the balanced flow?

We require control fields that are effectively independent (in the sense that error correlations between different fields are very small). So choosing the first control field requires - ideally - that none of the remaining control fields will project onto it. This requirement may be regarded as constraining the choice of the remaining control fields, but not the first; as previously noted, we may subtract the parts of the remaining control fields that do project onto the first control field, and work in terms of the residuals as new control fields - a procedure that clearly could be applied to the $(N+1)$th control field in terms of the N already chosen.

Note that the field we use to characterise the balanced flow may be invertibly transformed without affecting its suitability. For example, we can represent the rotational flow by either vorticity or streamfunction. In assessing the suitability of any candidate control field, any such invertible transformation makes no difference.

A simple geostrophic adjustment problem is described in Appendix 2. This shallow-water problem indicates on which horizontal scales an initial geostrophic imbalance will result mainly in adjustment of the rotational wind field to the initial pressure (or mass) field, and on which scales mainly in adjustment of the mass field to the initial rotational wind field. For

large horizontal scales, and small layer depth, the final balanced state corresponds closely to the initial mass field - i.e. the rotational wind adjusts to the pressure. On the other hand, for small horizontal scales, large layer depth, and in the tropics, the final balanced state corresponds closely to the rotational wind field - i.e. the pressure adjusts to the rotational wind. Under intermediate conditions, and at intermediate scales, mutual adjustment occurs.

To the extent that geostrophic adjustment is relevant to the choice of control fields, the suggestion is that pressure is a better choice on large horizontal scales and rotational wind is a better choice on small horizontal scales. Making different choices of control field for different scales would be difficult, but these results may be helpful in guiding our choice. For example, if we took the view that large horizontal scales are well-resolved, and so robust in the assimilation process, then we might choose rotational wind as control field because it will treat geostrophic adjustment at smaller, less well resolved scales better.

Allowing vertical structure in the geostrophic adjustment problem gives a somewhat different perspective. Solution in this case (see Appendix 2) shows that shallow-water depth corresponds - as expected - to vertical scale. Since the dominant vertical and horizontal scales H and L in quasi-geostrophic flow are approximately in the ratio f/N of the Coriolis and buoyancy frequencies, the solution (2.65) and (2.66) suggests that the mutual adjustment scenario is important.

In the adjustment problems considered in Appendix 2, PV is conserved irrespective of scale, so in all cases the final PV equals the initial PV. So on this criterion, PV is the best choice of control field (Cullen 2002a).

How accurately can we "invert" to calculate a well-balanced PF state?

We can invert the rotational wind, level by level, to give pressures, using the linear balance equation. In principle we can allow for boundary-layer friction; indeed, this is coded but has never been made to work (see Dance and Roulstone (2003) for discussion). We could perhaps improve on the balance by using a linearized nonlinear balance equation. But it has not been possible to put all orographic terms in, for our sloping coordinates, so balance over orography is imperfect. (These difficulties also are discussed by Dance and Roulstone (2003).) If we calculate temperatures hydrostatically from the vertical pressure differences, the rms

errors are much larger than actual temperature errors. This has been ascribed to unbalanced rotational wind increments with small vertical scales which are being inappropriately treated as balanced, but it could partly reflect a more basic difficulty with the concept of balanced pressure - see Appendix 3. We can get a better estimate of the balanced pressure field by applying a vertical regression, but the resulting pressure field then is not in balance with the wind field. [Another difficulty with the "balanced pressure" approach is that increments in the stratosphere are typically analysed as largely ageostrophic. See Ingleby (2001).]

If pressure (or height) is used as control field, we can calculate winds geostrophically; indeed, the first HIRLAM 3D-Var worked that way. But difficulties exist in the tropics, as the Coriolis parameter becomes small. Winds could be calculated from the nonlinear balance equation (possibly linearised), but section 7.6 of Daley (1991) suggests that difficulties would be encountered in this approach also.

PV can be inverted for the rotational wind - see papers by Tim Payne (1999). Mike Cullen has suggested using a streamfunction based on PV as control field, and coded it for the ECMWF spectral model. But nobody has yet gone beyond using simple geostrophic balance. Various possibilities are discussed in Appendix 4.

All the possible control fields can give pressure (or height) and rotational wind, as discussed above. It would be possible (and is desirable) to carry the inversion further: to evaluate associated divergent winds and vertical velocities (which might be identifed with the secondary circulations of quasi-geostrophic models). Derber and Bouttier (1999) showed that it is advantageous to derive balanced divergent wind increments from the rotational wind (they used a horizontal scale dependent regression in spectral space). We could implement a similar scheme; putting in horizontal scale dependence would be difficult, but we could for instance put in a dependence on boundary layer drag coefficients. More appealing would be a dynamically-based calculation of balanced divergent wind and vertical motion (e.g. from the quasi-geostrophic omega equation or a more accurate relative). This is being investigated by Ian Roulstone; see also Appendix 4. In the present state of knowledge, the difficulties with the approach seem to be about the same for each of our three choices of balanced control field.

Balanced contributions to other fields (moisture and ozone) could and probably should also be calculated. This is the same for all three choices of balanced control field.

How well can we model the 3D-error structure using our horizontal and vertical transforms?

There is a long heritage of modelling streamfunction and height error covariances. (Pressure in our height coordinate will behave like height in a pressure coordinate.) PV is nonlinear, so PV increments will have terms proportional to the linearisation state stability and vorticity. It is hard to work out if this will have a significant effect. (Mike Cullen is using a QG PV increment which does not have this dependence on the linearisation state.)

How difficult are the transforms to code?

We must code the control-field-to-model transform (U), its adjoint (U_hat), and its inverse (T). U and U_hat have to be efficient, since they are done within the variational inner-loop.

Using rotational wind was relatively easy (it's done). To make the U-transform easier (since that and its adjoint are more important than the T-transform), we choose to use streamfunction as control field (rather than vorticity or some other invertible relative).

Using pressure would be similarly easy.

The PV transforms are detailed in Tim Payne's notes. They appear considerably more complicated, and would require a 3D-solver. (Mike Cullen's (2002a) implementation is based on the ECMWF spectral semi-implicit model, splitting the solver into 2D problems using a basic state, and solving them spectrally. He mentions computational difficulties related to large condition numbers which are exacerbated by the use of a Lorenz grid.)

Conclusions

Streamfunction is an adequate balanced control field, and is probably better than pressure. Neither is appropriate as a control field on all scales, but a vertical regression procedure mitigates this defect and implementation is reasonably straightforward. A PV-based balanced control field is theoretically better than either streamfunction or pressure - it is appropriate at all scales - but it is more difficult to implement. We do not plan to develop this for the time being.

Using PV would not necessarily improve the accuracy of the balance achieved by "inversion" of the balanced control field to a perturbation state. Our higher priority is to improve this, to get balanced divergent and vertical motions, if this is possible.

Various other definitions of balance are being considered in research mode; see Appendix 4. Some difficulties with the concept of geostrophic pressure are discussed in Appendix 3.

3. Unbalanced hydrostatic control fields

After choosing the balanced control field, we need two others to define the unbalanced modes of a hydrostatic PE model. In terms of forecast errors, these two remaining control fields should be uncorrelated with the balanced control field and with each other. (If they are not, the assumed block-diagonal form of the covariance matrix $\mathbf{B}$ is vitiated). One way of promoting the desired uncorrelation is to choose one unbalanced control field to be simply the deviation from a calculated balanced component. For example, in the present procedure the balanced control field is streamfunction, and from it (as described in section 2) a balanced pressure is computed. An unbalanced pressure is then calculated by subtracting the balanced pressure from the pressure increment itself, and this unbalanced pressure is used as the first unbalanced control field. If pressure were the balanced control field, then the corresponding choice of first unbalanced control field would be the streamfunction of the unbalanced flow. In the case of a PV control field, the first unbalanced control field would be "anti-PV" (implying pressure and rotational wind increments such that the PV increment is zero). See Appendix 4 for discussion of specific cases.

The second unbalanced control field is part (currently all) of the divergent wind, which we can represent by an (unbalanced) velocity potential.

We might allow the total mass field, just as well as the balanced *flow*, to act as predictor for the "balanced" divergence. The divergent wind control field itself would then be the deviation from this balanced divergence.

In a hydrostatic formulation we can now calculate the hydrostatic (virtual) potential temperature, and the vertical motion (or the unbalanced vertical motion if a "balanced" vertical motion has been calculated as previously described).

4. Non-hydrostatic control fields

We need two extra control fields to complete the set for a (dry) non-hydrostatic model. One represents the deviation from the hydrostatic relationship of the (virtual) potential

temperature and the pressure. In the original design of Var we used a non-hydrostatic pressure field for this (alternatively a potential temperature field could be used). The second is a non-hydrostatic vertical motion. These are both deviations from the fields calculated using the hydrostatic control variables.

We judge that these control fields are unlikely to explain significant error variance. So, in line with our eigenvector expansion analogy, we truncate the series and omit these control fields.

5. Total moisture increment control field

We hypothesise that the most significant error variance concerns errors in the total moisture, independent of whether it is condensed or not. So we want the first moist control field to represent this. We also need it to be uncorrelated with the hydrostatic control fields; we have already discussed (see section 2) the possibility of calculating a geostrophically-balanced contribution.

The initial design of VAR used a total relative humidity (i.e. q_t/q_sat) increment (although in many places only the vapour is considered in the current code). Studies had shown some correlation of q and T errors near saturation, but generally less correlation of relative humidity and T errors. rh_prime was therefore considered to be the better choice of independent control field.

A more flexible approach (similar in rationale to that currently used for pressure) is to predict a contribution q_t_prime_T from the temperature increments, and to only represent the residual by the control field. The coefficients in this "q-T regression" can be a function of the Linearisation State:

q_t_prime_T = 0 (away from saturation)
q_t_prime_T = (dq_sat/dT) * T_prime (near saturation).

Once the work to derive a balanced vertical motion comes to fruition, we can extend this approach so as to calculate a predicted q_t_prime_w. Physically, the relationship exists because usually there is a large q-gradient in the vertical. Changes to the vertical

advection therefore change q. A possible simple relationship could be obtained if we assume an advective time-scale dt (∼1 hour perhaps?), and calculate the vertical gradient from the linearisation state. Then

q_t_prime_w = (dq/dz) * w_prime * dt.

Alternatively one could determine average correlation coefficients between w_prime and q_prime using the NMC method. (Mike Cullen says that global average coefficients like this only explain about 5% of the q_prime variance in the ECMWF system.)

When it comes to the statistical modelling of control variable covariances, q is perhaps not ideal in that it has a wide range of variances. An alternative is to normalise by q_sat. The U_p transform (the parameter part of the U transform) for moisture then becomes

q_t_prime = q_t_prime_T + q_t_prime_w + q_sat * mu

N.B. all the above U_p relationships have to be linear in the primed variables.

6. Condensation control fields

When we need increments for the full set of control fields, we need hypothesised relationships which predict increments for each from the single "total moisture" increment. If needed, these might include increments to precipitation rate, cloud water, cloud ice, and cloud amount. These relationships then imply a covariance model for the errors in the various fields (Lorenc 2000).

If we wanted a complete, non-singular, description of this full covariance matrix, we would need to specify additional control fields describing the possible deviations of the errors from the modelled relationships (e.g. cloud water increasing while water vapour decreases). Such effects are never likely to be significant - we do not have independent collocated observations of the various fields which are accurate enough to measure deviations from the relationships. So again we truncate the series and leave them out.

7. Need we bother with uncorrelation? - The alpha control field

Thus far we have used the analogy of eigenvector expansion to design our U_p and T_p transform. This gives us an ordered sequence explaining maximum variance, error independence, and easy invertibility. But if we are willing to give up these properties, we can use

$$x = Uv$$

$$B = \left\langle xx^T \right\rangle = U \left\langle vv^T \right\rangle U^T$$

to define our background covariance model using any U for which we have plausible physical hypotheses. For instance we could have the first control field defining balanced increments, and then three (i.e. one too many) control fields defining unbalanced rotational wind, unbalanced mass field, and divergence. (The first (1993) ECMWF 3D-Var implementation did this.)

We have used this approach to define additional "EotD" control fields. To the control fields described in earlier sections, we add a control field which defines a slowly varying position-dependent scaling for "Errors of the Day" modes which might be obtained from an error-breeding cycle. Since the normal control fields can already describe the complete space of hydrostatic increments (except for spectral truncations), the EotD field cannot be uncorrelated with them. This makes defining the inverse transform (the T transform) difficult - we have not attempted it. So we cannot obtain or check coefficients in the new combined model for covariances by analysis of actual increment or error files (e.g. the NMC method).

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Appendices

1 Some mathematical details (Appendix 1)

Let $\mathbf{x}$ be the state that represents the best compromise between the the available observations $\mathbf{y}^o$ and the model's background state $\mathbf{x}^b$ at the initial time. The vectors $\mathbf{x}$ and $\mathbf{x}^b$ have the same (very large) dimension; they contain - in some agreed order - all the model's main prognostic fields at all the gridpoints of the model. $\mathbf{x}^b$ is determined by a previous integration of the numerical model, and so may be regarded as known, while $\mathbf{x}$ is the unknown vector that we seek. The difference vector $\mathbf{x}-\mathbf{x}^b$ is the vector of *increments*. The (known) vector $\mathbf{y}^o$ will be different in nature from $\mathbf{x}$ and $\mathbf{x}^b$ - almost certainly as regards length, and probably as regards content: the number of observations bears little relation to the number or location of model gridpoints, and the observations need not be of the same quantities as the model's fields (although the observed quantities must be expressible in terms of them).

Bayesian arguments (Lorenc (1988) - Gaussian error distributions are assumed) show that the desired model state $\mathbf{x}$ minimises a single dimensionless number $J(\mathbf{x})$ called the penalty and given by

$$J(\mathbf{x}) = J^b(\mathbf{x}) + J^o(\mathbf{x}), \tag{1.1}$$

where $J^b(\mathbf{x})$ is a measure of the departure of $\mathbf{x}$ from the background state $\mathbf{x}^b$ and $J^o(\mathbf{x})$ is a measure of the departure of $\mathbf{x}$ from the observations $\mathbf{y}^o$. In terms of matrices $\mathbf{B}$, $\mathbf{E}$ and $\mathbf{F}$ - soon to be defined - the precise forms of $J^b(\mathbf{x})$ and $J^o(\mathbf{x})$ are (see Lorenc *et al.* (2000)):

$$J^b(\mathbf{x}) = \frac{1}{2}\left(\mathbf{x}-\mathbf{x}^b\right)^T \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}^b\right); \tag{1.2}$$

$$J^o(\mathbf{x}) = \frac{1}{2}\left(\mathbf{y}(\mathbf{x})-\mathbf{y}^o\right)^T \left(\mathbf{E}+\mathbf{F}\right)^{-1}\left(\mathbf{y}(\mathbf{x})-\mathbf{y}^o\right). \tag{1.3}$$

The factors of 1/2 in (1.2) and (1.3) are introduced solely for later algebraic convenience. Vectors are understood to be column vectors (e.g. $\left(\mathbf{x}-\mathbf{x}^b\right)$) and superscript T means transposition - so that $\left(\mathbf{x}-\mathbf{x}^b\right)^T$ is a row vector.

Like J, both J^b and J^o are single dimensionless numbers; the definitions of the matrices $\mathbf{B}$, $\mathbf{E}$ and $\mathbf{F}$ ensure this. Consider first the expression (1.3) for J^o. The matrix $\mathbf{E}$ is the instrumental error covariance matrix and $\mathbf{F}$ is the interpolation error covariance matrix. The issue of interpolation errors arises because $\mathbf{y}(\mathbf{x})$ in (1.3) is the model-predicted observation (from the model value of $\mathbf{x}$) corresponding to the real observation $\mathbf{y}^o$. Since $\mathbf{y}^o$ will

almost certainly not correspond to any model gridpoint, interpolation to the location of each observation is necessary. In this account we are concerned in detail with J^b rather than J^o.

The matrix $\mathbf{B}$ which appears in the expression (1.2) for J^b is the model's background error covariance matrix. Its definition (assuming no model bias) is

$$\mathbf{B} = \left\langle \left(\mathbf{x}^b - \mathbf{x}^t\right) \left(\mathbf{x}^b - \mathbf{x}^t\right)^T \right\rangle . \tag{1.4}$$

Here $\mathbf{x}^t$ is the vector of the actual (true) values at the locations of the gridpoints, and $\langle\rangle$ represents an ensemble average (in the Bayesian sense). If the model is biased then

$$\left\langle \mathbf{x}^b - \mathbf{x}^t \right\rangle \neq 0 \tag{1.5}$$

and the definition of $\mathbf{B}$ becomes (strictly)

$$\mathbf{B} = \left\langle \left(\mathbf{x}^b - \mathbf{x}^t - \left\langle \mathbf{x}^b - \mathbf{x}^t \right\rangle\right) \left(\mathbf{x}^b - \mathbf{x}^t - \left\langle \mathbf{x}^b - \mathbf{x}^t \right\rangle\right)^T \right\rangle . \tag{1.6}$$

In either the biased or the unbiased case, $\mathbf{B}$ is a symmetric matrix. (The correlation between the error in variable I at gridpoint i with the error in variable J at gridpoint j is clearly the same as the correlation between the error in variable J at gridpoint j with the error in variable I at gridpoint i.) $\mathbf{B}$ is a matrix of correlations rather than correlation coefficients; hence the physical dimensions of each element are those of $\mathbf{x}^2$, so J^b is dimensionless.

If model errors in different variables and at different gridpoints were uncorrelated, then $\mathbf{B}$ would be the diagonal matrix of the error variances σ_m^2 of each variable at each gridpoint. $\mathbf{B}^{-1}$ would then be the diagonal matrix of the reciprocals of σ_m^2, and J^b would consist of terms of the form $\left(x_m - x_m^b\right)^2 / 2\sigma_m^2$. This special case is useful in a mnemonic sense regarding the form of J^b, but the non-zero off-diagonal elements of $\mathbf{B}$ are in practice crucial in expressing the spatial coherence scale of model error.

So far in this Appendix, we have assumed that the vector $\mathbf{x}$ represents the usual model quantities - the "main prognostic fields". In this case, many of the off-diagonal elements of $\mathbf{B}$ represent non-zero error correlations between different fields. The goal of the parameter transform (the T_p transform) is to introduce new control fields whose errors are mutually uncorrelated, and hence to reduce $\mathbf{B}$ to a block diagonal form (each block corresponding to the error covariance structure of one of the control fields). This is both mathematically desirable and physically reasonable. From now on, we assume that reduction of $\mathbf{B}$ to block diagonal form has been achieved by an appropriate parameter transform as discussed in the

main text. In other words, we now assume that the vector $\mathbf{x}$ represents the new control fields (errors in which are ideally uncorrelated) and that $\mathbf{B}$ is the block diagonal covariance matrix appropriate to them. [This admits the possibility of different covariance behaviours being associated with different control fields. For example, the space scale of error covariance for a truly unbalanced control field might be very much less than for a balanced control field.]

In the minimization of J (and in the determination of the vector $\mathbf{x}$ that corresponds to that minimum), information about the gradients of J with respect to the individual components of $\mathbf{x}$ is needed. What is required is $\partial J/\partial x_m$ for each component x_m of $\mathbf{x}$, or, in a more concise notation, the gradient vector $\partial J/\partial \mathbf{x}$. [Use of new control fields has not altered the minimization problem, but has eased it by reducing $\mathbf{B}$ to block diagonal form.]

The background error term J^b given by (1.2) is a quadratic form in the elements of $\mathbf{x}-\mathbf{x}^b$, the coefficients being determined by the elements of the inverse of $\mathbf{B}$. Simple rules for the differentiation of quadratic forms $\mathbf{x}^T\mathbf{S}\mathbf{x}$ are readily derived. Consider

$$Q = \mathbf{x}^T\mathbf{S}\mathbf{x} = \sum_{k=1}^{N}\sum_{l=1}^{N} x_k S_{kl} x_l = x_k S_{kl} x_l \,. \tag{1.7}$$

Here $\mathbf{x}$ is a vector of length N and $\mathbf{S}$ is a symmetric $N \times N$ matrix. The summations extend from k, $l = 1$ to k, $l = N$; and in the right-hand member of (1.7) they are implied by the usual convention of summation over repeated suffices. Upon noting that $\partial x_k/\partial x_j = \delta_{jk}$ ($\delta_{jk} = 1$ if $k = j$; $\delta_{jk} = 0$ if $k \neq j$) differentiation w.r.t. x_j gives

$$\frac{\partial Q}{\partial x_j} = \frac{\partial x_k}{\partial x_j} S_{kl} x_l + x_k S_{kl} \frac{\partial x_l}{\partial x_j} = \delta_{jk} S_{kl} x_l + x_k S_{kl} \delta_{jl} = S_{jl} x_l + S_{kj} x_k \,. \tag{1.8}$$

By the symmetry of $\mathbf{S}$, $S_{kj} = S_{jk}$. Since both k and l are dummy suffices in (1.8) we have

$$\frac{\partial Q}{\partial x_j} = S_{jl} x_l + S_{jk} x_k = 2 S_{jl} x_l \;\; \Rightarrow \;\; \frac{\partial Q}{\partial \mathbf{x}} = 2\mathbf{S}\mathbf{x} \,. \tag{1.9}$$

A second differentiation now gives

$$\frac{\partial^2 Q}{\partial x_i \partial x_j} = 2 S_{jl} \frac{\partial x_l}{\partial x_i} = 2 S_{jl} \delta_{il} = 2 S_{ji} = 2 S_{ij} \,. \tag{1.10}$$

The matrix of the second derivatives of a quadratic form Q is simply $2\times$the matrix associated with Q. This matrix of the second derivatives is called the Hessian of Q. With an appropriate understanding of what is meant by $\partial^2/\partial \mathbf{x}^2$, we may write concisely

$$Hess[Q] = \frac{\partial^2 Q}{\partial \mathbf{x}^2} = 2\mathbf{S} \,. \tag{1.11}$$

Application of slight extensions of (1.9) and (1.11) to (1.1), noting (1.2) and (1.3), gives

$$\frac{\partial J}{\partial \mathbf{x}} = \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}^b\right) + \mathbf{H}^T\left(\mathbf{E}+\mathbf{F}\right)^{-1}\left(\mathbf{H}\mathbf{x}-\mathbf{y}^o\right) \tag{1.12}$$

in which the linear relation $\mathbf{y} = \mathbf{H}\mathbf{x}$ is assumed (for clarity). Hence

$$\frac{\partial^2 J}{\partial \mathbf{x}^2} = \mathbf{B}^{-1} + \mathbf{H}^{\mathbf{T}}\left(\mathbf{E}+\mathbf{F}\right)^{-1}\mathbf{H}. \tag{1.13}$$

The required $\mathbf{x}$ is the solution of

$$\frac{\partial J}{\partial \mathbf{x}} = \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}^b\right) + \mathbf{H}^T\left(\mathbf{E}+\mathbf{F}\right)^{-1}\left(\mathbf{H}\mathbf{x}-\mathbf{y}^o\right) = 0, \tag{1.14}$$

which may be re-written as

$$\left[\frac{\partial^2 J}{\partial \mathbf{x}^2}\left(\mathbf{x}-\mathbf{x}^b\right) =\right] \quad \left(\mathbf{B}^{-1} + \mathbf{H}^T(\mathbf{E}+\mathbf{F})^{-1}\mathbf{H}\right)\left(\mathbf{x}-\mathbf{x}^b\right) = \mathbf{H}^T(\mathbf{E}+\mathbf{F})^{-1}\left(\mathbf{y}^o - \mathbf{H}\mathbf{x}^b\right). \tag{1.15}$$

This is a closed set of linear equations for the components of the increment $\mathbf{x}-\mathbf{x}^b$, there being as many components of $\partial J/\partial \mathbf{x}$ as there are of $\mathbf{x}$ and $\mathbf{x}^b$.

The *conditioning* of the system (1.15) depends on the range of eigenvalues of the Hessian matrix $\partial^2 J/\partial \mathbf{x}^2$ as given by (1.13). If the range of eigenvalues of the Hessian is small, then the problem is well posed (in the sense that the dependence of the solution on the adopted values of the known quantities is weak). If the range of eigenvalues of the Hessian is large, then the problem is ill posed (in the sense that the dependence of the solution on the adopted values of the known quantities is strong). [The condition number, C, which measures the sensitivity of solutions of $\mathbf{M}\mathbf{x} = \mathbf{b}$ to changes in $\mathbf{b}$, is $\|\mathbf{M}\|\,\|\mathbf{M}^{-1}\|$, where $\|\ \|$ is the chosen norm; see Newbery (1974) and Wilkinson (1965). In the L_2 (Euclidean) norm as applied to the vectors $\mathbf{b}$ and $\mathbf{x}$, $\|\mathbf{M}\| = \left[\text{max. eigenvalue of } \mathbf{M}^T\mathbf{M}\right]^{1/2}$, i.e. $\|\mathbf{M}\| = $ max. eigenvalue of $\mathbf{M}$ if $\mathbf{M}$ is symmetric. Since the eigenvalues of $\mathbf{M}^{-1}$ are the reciprocals of the eigenvalues of $\mathbf{M}$, C will be large, and the problem ill posed, if the range of eigenvalues of $\mathbf{M}$ is large.]

The conditioning of the system (1.14) thus depends on $\mathbf{E}$, $\mathbf{F}$ and $\mathbf{H}$ via the second term in the expression (1.13) for $\partial^2 J/\partial \mathbf{x}^2$, as well as on $\mathbf{B}$ via the first term in (1.13). [It can be shown that the Hessian $\partial^2 J/\partial \mathbf{x}^2$ is equal to the *analysis* error covariance matrix; see Daley (1991), chapter 2.] However, in a useful working approximation - certainly valid where there are no observations! - we may disregard the influence (via $\mathbf{E}$, $\mathbf{F}$ and $\mathbf{H}$) of the observations on the conditioning of the problem, and consider only the influence of the background error term $\mathbf{B}^{-1}$. The eigenvalues of $\mathbf{B}^{-1}$ are of course just the reciprocals of the eigenvalues of $\mathbf{B}$.

If errors are spatially homogeneous and isotropic, then the eigenvalues of $\mathbf{B}$ are equal to the Fourier or spherical harmonic amplitudes of the spatial covariance function. Further, the eigenvectors of $\mathbf{B}$ are simply sines and cosines (or harmonics on the sphere); see White and Healy (2003). While a homogeneous, isotropic model of errors is crude, these results show that the range of eigenvalues of $\mathbf{B}$ may be very large (zero eigenvalues are possible). Hence the condition number may be very large (even infinite, if zero eigenvalues occur), and the problem is ill posed. To overcome this, Lorenc (1988) proposed a transformation of the increment $\mathbf{x} - \mathbf{x}_b$ using the square root $\mathbf{U}$ of $\mathbf{B}$ defined by

$$\mathbf{B} = \mathbf{U}\mathbf{U}^T. \tag{1.16}$$

Given (1.16), we have

$$\mathbf{B}^{-1} = \left(\mathbf{U}^T\right)^{-1} \mathbf{U}^{-1}. \tag{1.17}$$

Hence

$$2J^b(\mathbf{x}) = \left(\mathbf{x} - \mathbf{x}^b\right)^T \mathbf{B}^{-1} \left(\mathbf{x} - \mathbf{x}^b\right) = \left(\mathbf{x} - \mathbf{x}^b\right)^T \left(\mathbf{U}^T\right)^{-1} \mathbf{U}^{-1} \left(\mathbf{x} - \mathbf{x}^b\right). \tag{1.18}$$

The transformation

$$\mathbf{x} - \mathbf{x}^b = \mathbf{U}\mathbf{X} \;\; (\Rightarrow \;\; \left(\mathbf{x} - \mathbf{x}^b\right)^T = \mathbf{X}^T\mathbf{U}^T) \tag{1.19}$$

reduces (1.18) to

$$2J^b(\mathbf{x}) = \mathbf{X}^T\mathbf{U}^T \left(\mathbf{U}^T\right)^{-1} \mathbf{U}^{-1}\mathbf{U}\mathbf{X} = \mathbf{X}^T\mathbf{X}. \tag{1.20}$$

This form gives a contribution

$$\frac{\partial^2 J^b}{\partial \mathbf{X}^2} = \mathbf{I}\,. \tag{1.21}$$

In terms of $\mathbf{X} = \mathbf{U}^{-1}\left(\mathbf{x} - \mathbf{x}^b\right)$, the problem is therefore well posed: the eigenvalues of the unit (diagonal) matrix $\mathbf{I}$ are all equal (to unity). We simply have to determine $\mathbf{U}$, the square root of $\mathbf{B}$, as defined by (1.16), in order to carry out the required preconditioning!

One procedure for constructing the square-root of a symmetric matrix such as $\mathbf{B}$ involves finding its eigenvectors and eigenvalues, and square-rooting the diagonal matrix of eigenvalues (Parrish and Derber 1992). The transformed vector $\mathbf{X}$ (see (1.19)) consists of scaled coefficients of a projection of the original vector $\mathbf{x} - \mathbf{x}_b$ onto the eigenvectors. It is very instructive to consider this procedure - although in practice (as we shall see) less precise methods are adopted. We first recall some relevant properties of a real symmetric matrix: the orthogonality of its eigenvectors, the reality of its eigenvalues, and a procedure for diagonalisation.

Eigenvector orthogonality and eigenvalue reality

Let $\mathbf{S}$ be an $N \times N$ real symmetric matrix; i.e. the element S_{ij} in row i and column j is real, and $S_{ji} = S_{ij}$ $[1 \leq i \leq N,\ 1 \leq j \leq N]$. Clearly, $\mathbf{S}$ is identically equal to its transpose $\mathbf{S}^T$. Suppose that $\mathbf{e}^p$ and $\mathbf{e}^q$ are (column) eigenvectors of $\mathbf{S}$ with eigenvalues λ^p and λ^q:

$$\mathbf{S}\mathbf{e}^p = \lambda^p \mathbf{e}^p; \tag{1.22}$$

$$\mathbf{S}\mathbf{e}^q = \lambda^q \mathbf{e}^q. \tag{1.23}$$

Manipulation of (1.22) and (1.23) and use of the reality and symmetry of $\mathbf{S}$ lead to

$$\left[\lambda^p - (\lambda^q)^*\right] (\mathbf{e}^q)^{*T} \mathbf{e}^p = 0. \tag{1.24}$$

Considering the case $p = q$ shows that all the eigenvalues must be real. Hence real eigenvectors may be identified. From (1.24) it also follows that the eigenvectors belonging to unequal eigenvalues are orthogonal:

$$(\mathbf{e}^p)^T \mathbf{e}^q = 0. \tag{1.25}$$

It can be shown that orthogonalization is possible within the subspace of eigenvectors belonging to equal eigenvalues (the Schmidt process for "degenerate" cases).

Optimality of truncated eigenvector expansions

An arbitrary column vector $\mathbf{v}$ of length N can be expressed as a linear combination of the N normalized eigenvectors of $\mathbf{S}$:

$$\mathbf{v} = \sum_{p=1}^{p=N} v_p \mathbf{e}^p. \tag{1.26}$$

Consider an approximation $\mathbf{u}^{(P)}$ to $\mathbf{v}$ as some linear combination of P $(< N)$ of the N normalized eigenvectors of $\mathbf{S}$:

$$\mathbf{u}^{(P)} = \sum_{p=1}^{p=P} u_p \mathbf{e}^p. \tag{1.27}$$

In view of the orthogonality (1.24) of the eigenvectors of $\mathbf{S}$, (1.26) and (1.27) imply

$$\left(\mathbf{v} - \mathbf{u}^{(P)}\right)^2 \equiv \left(\mathbf{v} - \mathbf{u}^{(P)}\right)^T \left(\mathbf{v} - \mathbf{u}^{(P)}\right) = \sum_{p=1}^{p=P} (v_p - u_p)^2 + \sum_{p=P+1}^{p=N} v_p^2 \,. \tag{1.28}$$

The most accurate approximation $\mathbf{u}^{(P)}$ to $\mathbf{v}$, in terms of mean square difference and hence variance explained, is therefore obtained by setting $u_p = v_p$ for all $p \leq P$. In other words, the approximation to $\mathbf{v}$ obtained by retaining only the first P terms of (1.26) is the most accurate of all linear combinations of the first P eigenvectors.

Diagonalization

Consider the matrix $\mathbf{E}$ whose *columns* are the *normalised* eigenvectors of $\mathbf{S}$. More specifically, let $\mathbf{E}$ be the matrix whose pth column is the normalised eigenvector $\mathbf{e}^p$ that belongs to the eigenvalue λ^p:

$$\mathbf{E} = \begin{pmatrix} e_1^1 & e_1^2 & e_1^3 & .. & e_1^N \\ e_2^1 & e_2^2 & e_2^3 & .. & e_2^N \\ e_3^1 & e_3^2 & e_3^3 & .. & e_3^N \\ : & : & : & : & : \\ e_N^1 & e_N^2 & e_N^3 & .. & e_N^N \end{pmatrix} \tag{1.29}$$

When the matrix $\mathbf{SE}$ is formed, the pth column of the product will contain the result of $\mathbf{S}$ acting on the pth column of $\mathbf{E}$, i.e. the result of $\mathbf{S}$ acting on $\mathbf{e}^p$, which is simply $\lambda^p \mathbf{e}^p$:

$$\mathbf{SE} = \begin{pmatrix} \lambda^1 e_1^1 & \lambda^2 e_1^2 & \lambda^3 e_1^3 & .. & \lambda^N e_1^N \\ \lambda^1 e_2^1 & \lambda^2 e_2^2 & \lambda^3 e_2^3 & .. & \lambda^N e_2^N \\ \lambda^1 e_3^1 & \lambda^2 e_3^2 & \lambda^3 e_3^3 & .. & \lambda^N e_3^N \\ : & : & : & : & : \\ \lambda^1 e_N^1 & \lambda^2 e_N^2 & \lambda^3 e_N^3 & .. & \lambda^N e_N^N \end{pmatrix} \tag{1.30}$$

By the orthogonality of the eigenvectors of $\mathbf{S}$, $\mathbf{E}^T\mathbf{E} = \mathbf{I}$ (since the i, j element in $\mathbf{E}^T\mathbf{E}$ is simply $\left(\mathbf{e}^i\right)^T \mathbf{e}^j = \delta_{ij}$, the eigenvectors having been normalised). By the same reasoning, the matrix $\mathbf{E}^T\mathbf{SE}$ is the diagonal matrix $\mathbf{L}$ of the eigenvalues of $\mathbf{S}$:

$$\mathbf{E}^T\mathbf{SE} = \mathbf{L} = \begin{pmatrix} \lambda^1 & 0 & 0 & .. & 0 \\ 0 & \lambda^2 & 0 & .. & 0 \\ 0 & 0 & \lambda^3 & .. & 0 \\ : & : & : & : & : \\ 0 & 0 & 0 & .. & \lambda^N \end{pmatrix} \tag{1.31}$$

The well-known result (1.31) gives a straightforward method for finding the square root of a symmetric matrix. The square root of a diagonal matrix $\delta_{ij}d_j$ is simply the diagonal

matrix $\delta_{ij}\sqrt{d_j}$; in particular

$$\sqrt{\mathbf{L}} = \begin{pmatrix} \sqrt{\lambda^1} & 0 & 0 & .. & 0 \\ 0 & \sqrt{\lambda^2} & 0 & .. & 0 \\ 0 & 0 & \sqrt{\lambda^3} & .. & 0 \\ : & : & : & : & : \\ 0 & 0 & 0 & .. & \sqrt{\lambda^N} \end{pmatrix} \tag{1.32}$$

Upon noting that $\mathbf{E}^T\mathbf{E} = \mathbf{I} \Rightarrow \mathbf{E}\mathbf{E}^T = \mathbf{I}$, it follows from (1.31) and (1.32) that

$$\mathbf{S} = \mathbf{E}\mathbf{L}\mathbf{E}^T = \mathbf{E}\sqrt{\mathbf{L}}\sqrt{\mathbf{L}}\mathbf{E}^T = \mathbf{E}\sqrt{\mathbf{L}}\left(\mathbf{E}\left(\sqrt{\mathbf{L}}\right)\right)^T, \tag{1.33}$$

i.e.

$$\mathbf{S} = \mathbf{R}\mathbf{R}^T \tag{1.34}$$

where

$$\mathbf{R} = \mathbf{E}\sqrt{\mathbf{L}} \tag{1.35}$$

$\mathbf{R}$ is the square root of $\mathbf{S}$ in the required sense for our pre-conditioning problem. Furthermore,

$$\mathbf{R} = \mathbf{E}\sqrt{\mathbf{L}} = \begin{pmatrix} e_1^1 & e_1^2 & e_1^3 & .. & e_1^N \\ e_2^1 & e_2^2 & e_2^3 & .. & e_2^N \\ e_3^1 & e_3^2 & e_3^3 & .. & e_3^N \\ : & : & : & : & : \\ e_N^1 & e_N^2 & e_N^3 & .. & e_N^N \end{pmatrix} \begin{pmatrix} \sqrt{\lambda^1} & 0 & 0 & .. & 0 \\ 0 & \sqrt{\lambda^2} & 0 & .. & 0 \\ 0 & 0 & \sqrt{\lambda^3} & .. & 0 \\ : & : & : & : & : \\ 0 & 0 & 0 & .. & \sqrt{\lambda^N} \end{pmatrix} \tag{1.36}$$

from which it is readily seen that $\mathbf{R}$ is the matrix whose pth column is simply $\sqrt{\lambda^p}\mathbf{e}^p$ (cf. (1.30) for $\mathbf{SE}$). Clearly, the inverse $\mathbf{R}^{-1}$ is the matrix whose qth *row* is $\left(\sqrt{\lambda^q}\right)^{-1}\left(\mathbf{e}^q\right)^T$.

These results may be applied straightforwardly to express the transformed variable $\mathbf{X} = \mathbf{U}^{-1}\left(\mathbf{x} - \mathbf{x}^b\right)$ (see (1.19)) in terms of the eigenvalues λ^n of $\mathbf{B}$ and the coefficients of the expansion of $\mathbf{x} - \mathbf{x}^b$ in terms of the eigenvectors of $\mathbf{B}$. If

$$\mathbf{x} - \mathbf{x}^b = \sum_{p=1}^{p=N} x_p \mathbf{e}^p, \tag{1.37}$$

then

$$\mathbf{X} = \mathbf{U}^{-1}\left(\mathbf{x} - \mathbf{x}^b\right) = \begin{pmatrix} x_1/\sqrt{\lambda^1} \\ x_2/\sqrt{\lambda^2} \\ x_3/\sqrt{\lambda^3} \\ : \\ x_N/\sqrt{\lambda^N} \end{pmatrix} \tag{1.38}$$

Thus the transformed vector $\mathbf{X}$ indeed consists of scaled coefficients of a projection of the original variables $\mathbf{x} - \mathbf{x}^b$ onto the eigenvectors of $\mathbf{B}$. If the projection of $\mathbf{x} - \mathbf{x}^b$ onto the eigenvectors is denoted by $\widetilde{\Delta\mathbf{x}}$, then $\mathbf{X} = \mathbf{L}^{-1/2}\widetilde{\Delta\mathbf{x}}$. [It is worth noting from (1.38) that the procedure will break down if any eigenvalue vanishes; we can re-condition cases in which the range of eigenvalues is large, but we cannot by this method redeem pathological cases.]

If errors are *homogeneous* and *isotropic*, the eigenvectors of $\mathbf{B}$ are sinusoids or spherical harmonics, and the associated eigenvalues are simply their coefficents in the Fourier decomposition of the single function that specifies the error covariance (see White and Healy 2003). For example, in a cyclic 1D Cartesian domain having repeat distance $2L$, the eigenvectors of $\mathbf{B}$ are just the sinusoids $\sin \pi mx/L$ and $\cos \pi mx/L$ ($m =$ integer) evaluated at the grid-points, and the eigenvalues of $\mathbf{B}$ (for both sine and cosine eigenvectors) are the coefficents of $\cos \pi mx/L$ in the discrete Fourier cosine expansion of the generic row of $\mathbf{B}$:

$$B_{1j} = \frac{b_0}{2} + \sum_{m=1}^{m=M} b_m \cos\left(2\pi mj/N\right). \tag{1.39}$$

The relevant eigenvector expansion of $\mathbf{x} - \mathbf{x}^b$ (cf. (1.37)) is a truncated Fourier series

$$\mathbf{x} - \mathbf{x}^b = \frac{x_0}{2} + \sum_{m=1}^{m=M} \left[x_m^c \cos\left(2\pi mj/N\right) + x_m^s \sin\left(2\pi mj/N\right)\right]. \tag{1.40}$$

In both (1.39) and (1.40), the upper limit in the sums is $M \equiv (N-1)/2$. The transformed variable (cf. (1.38)) is

$$\mathbf{X} = \mathbf{U}^{-1}\left(\mathbf{x} - \mathbf{x}^b\right) = \begin{pmatrix} x_0/\sqrt{b_0/2} \\ x_1^c/\sqrt{b_1} \\ x_1^s/\sqrt{b_1} \\ x_2^c/\sqrt{b_2} \\ x_2^s/\sqrt{b_2} \\ \vdots \\ \vdots \\ x_M^c/\sqrt{b_M} \\ x_M^s/\sqrt{b_M} \end{pmatrix} \tag{1.41}$$

The transformed vector $\mathbf{X}$ which re-conditions the equation for $\mathbf{x} - \mathbf{x}^b$ is in this case simply the discrete Fourier transform of $\mathbf{x} - \mathbf{x}^b$ modified by a systematic re-scaling of each term. It seems that this transform would have been a good move even if conditioning had not been an issue.

In reality, model errors are not homogeneous and isotropic (either as regards covariance or correlation). On the other hand we cannot calculate the eigenvectors of the real background error covariance matrix. This is not just because the matrix is too big to store, let alone manipulate; more fundamentally, the matrix itself is unknowable. Calculating it would require more forecast runs than we could ever make, plus complete accurate verification for each. What is more, the behaviour of errors is flow-dependent.

So we have to construct some sort of *model* of the covariances, based on physically reasonable hypotheses. A model based on a hypothesis of homogeneous and isotropic error has much to recommend it, but our scheme - described by Lorenc *et al.* (2000) - aims to do better by using a specification having assignable constants that can be determined by comparison with model errors using the "NMC method". [In this method, error fields and their statistics are estimated from the differences between 48- and 24-hour forecasts verifying at the same time.] The covariance model is based on physical hypotheses as much as on covariance statistics; we derive transforms physically in the first instance, and resort to statistics to determine assignable constants only when our physical insight is used up. See Lorenc *et al.* (2000) for further details.

2 A geostrophic adjustment problem (Appendix 2)

This example is taken from Lorenc (1979). Consider small-amplitude motion described by the $f-$plane shallow water equations with divergence damping. When linearised about a state of rest, the vorticity, divergence and continuity equations become

$$\frac{\partial \zeta}{\partial t} = -fD, \tag{2.42}$$

$$\frac{\partial D}{\partial t} = f\zeta - g\nabla^2 h - \mu\nabla^2 D, \tag{2.43}$$

$$\frac{\partial h}{\partial t} = -h_0 D\,. \tag{2.44}$$

Here ζ is the vorticity $(\partial v/\partial x - \partial u/\partial y)$, D is the divergence $(\partial u/\partial x + \partial v/\partial y)$, h is the deviation of the free surface from its (uniform) equilibrium height h_0, and μ is the divergence damping coefficent. This set of equations describes undamped geostrophic modes (which are stationary because of the absence of both mean flow and $\beta-$effect) and pairs of damped

propagating surface gravity modes. In terms of the streamfunction ψ we have $\zeta = \nabla^2\psi$, and (2.42) and (2.43) become

$$\frac{\partial}{\partial t}\nabla^2\psi = -fD, \tag{2.45}$$

$$\frac{\partial D}{\partial t} = f\nabla^2\psi - g\nabla^2 h - \mu\nabla^2 D. \tag{2.46}$$

The steady states of (2.44)-(2.46) ($\partial/\partial t = 0$) are geostrophic states obeying $D = 0$ (from (2.44) and (2.45)) and $\nabla^2\psi = (g/f)\nabla^2 h \Rightarrow \psi = gh/f$ (from(2.46)). The vorticity equation (2.45) and the continuity equation (2.44) together imply the conservation law

$$\frac{\partial}{\partial t}\left\{\nabla^2\psi - f\frac{h}{h_0}\right\} = 0, \tag{2.47}$$

which is a linearised form of potential vorticity conservation. [Note, however, that no relationship between ψ and h has yet been applied.]

Eq (2.47) makes the solution of geostrophic adjustment problems easy, so long as we are interested only in final (adjusted) states. Suppose that the initial state has streamfunction ψ_i and free-surface height deviation h_i, and that the final "adjusted" geostrophic state has steamfunction ψ_s and free-surface height deviation h_s. Necessarily $\psi_s = gh_s/f$, because the *final* state is in geostrophic balance, but the problem is trivial if the *initial* state is in geostrophic balance (since no evolution would then occur). From (2.47), the initial and final states are related by

$$\nabla^2\psi_s - \frac{f^2}{gh_0}\psi_s = \nabla^2\psi_i - \frac{f^2}{gh_0}\left(\frac{gh_i}{f}\right). \tag{2.48}$$

Now assume sinusoidal structure for ψ_i, h_i and ψ_s:

$$\psi_i = \widehat{\psi}_i \exp[i(kx + ly)] \tag{2.49}$$

and similarly for h_i and ψ_s. Substitution into (2.48) and re-arrangement gives

$$\widehat{\psi}_s = \alpha\widehat{\psi}_i + (1-\alpha)\frac{g\widehat{h}_i}{f}, \tag{2.50}$$

in which the key parameter α is defined as

$$\alpha \equiv \frac{k^2 + l^2}{k^2 + l^2 + (f^2/gh_0)} = \frac{1}{1 + \frac{f^2}{gh_0(k^2+l^2)}}. \tag{2.51}$$

According to (2.50) the adjustment is radically different in the two cases $\alpha \ll 1$ and $\alpha \simeq 1$. When $\alpha \ll 1$, the final state ψ_s is close to the geostrophic streamfunction gh_i/f. When

$\alpha \simeq 1$, the final state is close to the *initial* streamfunction ψ_i. In other words, for large horizontal scales and/or shallow layers, the rotational flow field adjusts to the initial mass field; but for small horizontal scales and/or deep layers, the mass field adjusts to the initial rotational flow field.

Eq (2.51) may be re-written as

$$\alpha = \frac{\lambda_R^2}{\lambda_R^2 + \lambda_{xy}^2}, \tag{2.52}$$

in which

$$\lambda_R = 2\pi\sqrt{\frac{gh_0}{f_0^2}} \tag{2.53}$$

is ($2\pi\times$) a Rossby radius of deformation, and λ_{xy} is related to the zonal wavelength $\lambda_x = 2\pi/k$ and the meridional wavelength $\lambda_y = 2\pi/l$ by

$$\lambda_{xy}^2 \equiv \frac{\lambda_x^2 \lambda_y^2}{\lambda_x^2 + \lambda_y^2}\,. \tag{2.54}$$

Eqs (2.52) and (2.54) show that $\alpha \ll 1$ requires the geometric mean of the zonal and the meridional wavelengths to be large; it is not enough just to have a large scale in one direction.

It is straightforward to extend this shallow water analysis to cases in which vertical structure is allowed. Consider a stratified Boussinesq fluid having mean density profile $\rho_0(z)$ and buoyancy frequency $N(z)$. The vorticity and divergence equations (2.45) and (2.46) remain formally unchanged, although height variation of all fields is now allowed, and gh is replaced by the quantity $\pi = p/\rho_0$, where p is the perturbation pressure:

$$\frac{\partial}{\partial t}\nabla^2\psi = -fD, \tag{2.55}$$

$$\frac{\partial D}{\partial t} = f\nabla^2\psi - \nabla^2\pi - \mu\nabla^2 D. \tag{2.56}$$

Equation (2.44) is superseded by the result of eliminating vertical velocity w and buoyancy b between the hydrostatic, thermodynamic and continuity equations in the forms

$$b = \frac{\partial \pi}{\partial z}, \tag{2.57}$$

$$\frac{\partial b}{\partial t} + N^2 w = 0, \tag{2.58}$$

$$D + \frac{1}{\rho_0}\frac{\partial}{\partial z}\left(\rho_0 w\right) = 0. \tag{2.59}$$

The required expression is

$$\frac{\partial}{\partial t}\left[\frac{\partial}{\partial z}\left(\frac{\rho_0}{N^2}\frac{\partial \pi}{\partial z}\right)\right] = \rho_0 D. \tag{2.60}$$

From (2.57) and (2.58) we can also derive the condition on π at rigid horizontal surfaces as

$$\frac{\partial}{\partial t}\left(\frac{\partial \pi}{\partial z}\right) = 0. \tag{2.61}$$

From (2.55) and (2.60) follows the conservation law

$$\frac{\partial}{\partial t}\left\{\nabla^2\psi + \frac{f}{\rho_0}\frac{\partial}{\partial z}\left(\frac{\rho_0}{N^2}\frac{\partial \pi}{\partial z}\right)\right\} = 0. \tag{2.62}$$

The conserved quantity in (2.62) is reminiscent of quasi-geostrophic potential vorticity, but no relationship between ψ and π has yet been enforced.

For the *final* (adjusted) state we have $\psi_s = \pi_s/f$, and applying (2.62) at the initial and final states gives

$$\nabla^2\psi_s + \frac{f^2}{\rho_0}\frac{\partial}{\partial z}\left(\frac{\rho_0}{N^2}\frac{\partial \psi_s}{\partial z}\right) = \nabla^2\psi_i + \frac{f^2}{\rho_0}\frac{\partial}{\partial z}\left(\frac{\rho_0}{N^2}\frac{\partial}{\partial z}\left[\frac{\pi_i}{f}\right]\right). \tag{2.63}$$

This should be compared with (2.48). In a familiar approximation (the isothermal case is also tractable), we neglect the height variation of the reference density $\rho_0(z)$, and assume uniform N; then (2.63) becomes

$$\nabla^2\psi_s + \frac{f^2}{N^2}\frac{\partial^2 \psi_s}{\partial z^2} = \nabla^2\psi_i + \frac{f^2}{N^2}\frac{\partial^2}{\partial z^2}\left(\frac{\pi_i}{f}\right). \tag{2.64}$$

Posing spatial structure of the form $\exp[i(kx+ly)]\cos\left(\frac{M\pi z}{H}\right)$ (so as to satisfy (2.61) at rigid horizontal boundaries at $z = 0, H$) we find

$$\widehat{\psi_s} = \gamma\widehat{\psi_i} + (1-\gamma)\frac{\widehat{\pi}_i}{f}, \tag{2.65}$$

with

$$\gamma = \frac{1}{1 + \frac{f^2M^2\pi^2}{N^2H^2(k^2+l^2)}}. \tag{2.66}$$

These results are directly comparable with (2.50) and (2.51): $g\widehat{h}_i$ is replaced by $\widehat{\pi}_i$, and γ is formally the same as α, but $(NH/M\pi)^2$ replaces gh_0. Thus, internal gravity waves can indeed be identified with shallow water modes for appropriately small depths h_0. This is consistent with established notions of "equivalent depth". For internal gravity waves, it is clear that γ decreases as the mode number M increases. So the adjustment will be increasingly of the flow to the mass field as the vertical scale of internal gravity waves decreases.

Extension to the case of a compressible stratified fluid is also straightforward (at least with the hydrostatic approximation). The PV conservation law (2.62) is unchanged, and in the rigid-surface boundary condition (2.61) $\partial\pi/\partial z$ is simply replaced by $\partial\pi/\partial z - N^2\pi/g$.

3 The concept of balanced pressure (Appendix 3)

In geophysical fluid dynamics it is usual to define balanced *flow*s corresponding to given pressure fields, rather than balanced *pressure fields* corresponding to given flows. Examples are the well-known geostrophic, gradient and cyclostrophic winds, which are each related in a clearly defined way to given pressure (or height) fields.

Geostrophic adjustment problems (such as the one described in Appendix 2) have led to notions of streamfunction-constrained initialization and geopotential-constrained initialization; see Daley (1991). The idea of a balanced *geostrophic pressure* is traceable to Parrish and Derber's (1992) choice of analysis variables, which includes a geostrophic height field. In this Appendix we examine the concept of geostrophic pressure and note some difficulties in its use to define a control field.

Geostrophic balance between a wind field $\mathbf{v}$ and a pressure field p is expressed by the vector equation

$$-\rho f\mathbf{k}\times\mathbf{v} - \nabla_2 p \;=\; 0\,. \tag{3.67}$$

Here $\rho =$ density, f is the Coriolis parameter, $\mathbf{k}$ is unit vector in the upward vertical direction, and ∇_2 is the horizontal gradient operator. The terms $-\rho f\mathbf{k}\times\mathbf{v}$ and $-\nabla_2 p$ in (3.67) represent the horizontal parts of the Coriolis force and the pressure gradient force (per unit volume).

For any (once differentiable) pressure field p, (3.67) may be used to define a corresponding geostrophic wind field $\mathbf{v}_G$ as

$$\mathbf{v}_G = \frac{1}{\rho f}\mathbf{k}\times\nabla_2 p\,. \tag{3.68}$$

As an approximation to the real wind $\mathbf{v}$, (3.68) is poor close to the equator, but as a *definition* of $\mathbf{v}_G$ it fails only at the equator (where $f = 0$), and may be redeemed even there if $\partial p/\partial\phi$ behaves accommodatingly.

Suppose we attempt to use (3.67) to define a *geostrophic pressure* field p^G for any given velocity field $\mathbf{v}$:

$$\nabla_2 p^G = -\rho f\mathbf{k}\times\mathbf{v}\,. \tag{3.69}$$

This is satisfactory only if it defines $\nabla_2 p^G$ as a true horizontal gradient. In particular, $\nabla_2 p^G$ must be irrotational, i.e. $\mathbf{k} \cdot \nabla_2 \times \left(\nabla_2 p^G\right) = 0$. So (3.69) is satisfactory only if $\mathbf{k} \cdot \nabla_2 \times (\rho f \mathbf{k} \times \mathbf{v}) = 0$, which (by use of the almost obvious identity $\mathbf{k} \cdot \nabla \times (\mathbf{k} \times \mathbf{a}) = \nabla \cdot \mathbf{a}$, valid for any once-differentiable vector field $\mathbf{a}$) reduces to

$$\nabla_2 \cdot (\rho f \mathbf{v}) = 0. \tag{3.70}$$

Condition (3.70) will not generally be obeyed. [It requires non-divergent flow in the case of constant ρf.] Thus (3.69) is not a satisfactory definition of a geostrophic pressure field.

The difficulty may be overcome by taking the horizontal divergence ($\nabla_2 \cdot$) of (3.69):

$$\nabla_2^2 p^G = -\nabla_2 \cdot (\rho f \mathbf{k} \times \mathbf{v}) \,, \tag{3.71}$$

and using this 2D Poisson equation to *define* p^G (requiring, for example, continuity of p^G over a spherical surface). This is what is done in practice.

It should be noted that (3.71) is a completely new definition of p^G. This must indeed be so, since we have shown that (3.69) is not generally satisfactory, but it is revealing to examine why (3.71) works but (3.69) doesn't. Consider (3.69) in the augmented form

$$\nabla_2 p^G = -\rho f \mathbf{k} \times \mathbf{v} \; + \mathbf{k} \times \nabla_2 F, \tag{3.72}$$

in which F is any once-differentiable function. Taking the divergence of (3.72) still gives (3.71) because $\nabla_2 \cdot (\mathbf{k} \times \nabla_2 F) = 0$, i.e. $\mathbf{k} \times \nabla_2 F$ is non-divergent. But it is the term $\mathbf{k} \times \nabla_2 F$ in (3.72) which enables the irrotationality of $\nabla_2 p^G$ to be maintained; from (3.72) we have

$$\mathbf{k} \cdot \nabla_2 \times \nabla_2 p^G = \mathbf{k} \cdot \nabla_2 \times [\mathbf{k} \times (\nabla_2 F - \rho f \mathbf{v})] = \mathbf{k} \cdot \nabla_2 \cdot (\nabla_2 F - \rho f \mathbf{v}) \,. \tag{3.73}$$

Hence the irrotationality of $\nabla_2 p^G$ can be assured by choosing F such that $\nabla_2^2 F = \nabla_2 \cdot (\rho f \mathbf{v})$.

As noted in section 2, difficulties have been experienced with the vertical consistency of the geostrophic pressures p^G calculated for different levels: the temperature structure implied by hydrostatic balance is unsatisfactory. We now show that such problems are an almost inevitable consequence of using the 2D Poisson equation (3.71) to define p^G. Differentiation of (3.71) w.r.t. height z gives

$$\nabla_2^2 \left(\frac{\partial p^G}{\partial z} \right) = -\nabla_2 \cdot \left(f \mathbf{k} \times \frac{\partial}{\partial z} (\rho \mathbf{v}) \right) . \tag{3.74}$$

Suppose that p^G is required to be in hydrostatic balance with the density field ρ, i.e.

$$\frac{\partial p^G}{\partial z} = -\rho g. \tag{3.75}$$

Use of (3.75) in (3.74) gives

$$\nabla_2 \cdot \left\{ \nabla_2 (\rho g) - f\mathbf{k} \times \frac{\partial}{\partial z} (\rho \mathbf{v}) \right\} = 0 \,, \tag{3.76}$$

which will be obeyed only if the vector in the curly brackets is non-divergent, i.e.

$$\nabla_2 (\rho g) - f\mathbf{k} \times \frac{\partial}{\partial z} (\rho \mathbf{v}) = \mathbf{k} \times \nabla_2 G, \tag{3.77}$$

for some once-differentiable function G. Condition (3.77) will *not* in general be obeyed; instead, we will have a Helmholtz decomposition of the form

$$\nabla_2 (\rho g) - f\mathbf{k} \times \frac{\partial}{\partial z} (\rho \mathbf{v}) = \mathbf{k} \times \nabla_2 G + \nabla_2 H, \tag{3.78}$$

in which H is a once-differentiable function. This may be demonstrated from the momentum equation in the form

$$\rho \frac{D\mathbf{v}}{Dt} + \rho f \mathbf{k} \times \mathbf{v} + \nabla_2 p = \rho \mathbf{F}_2 \tag{3.79}$$

(in which $\mathbf{F}_2$ is the horizontal frictional force per unit mass). By differentiating (3.79) w.r.t. height z and using the hydrostatic equation (3.75) [but for p rather than p^G] we obtain

$$\nabla_2 (\rho g) - f\mathbf{k} \times \frac{\partial}{\partial z} (\rho \mathbf{v}) = \frac{\partial}{\partial z} \left(\rho \left[\frac{D\mathbf{v}}{Dt} - \mathbf{F} \right] \right) . \tag{3.80}$$

Comparison with (3.78) then gives

$$\mathbf{k} \times \nabla_2 G + \nabla_2 H = \frac{\partial}{\partial z} \left(\rho \left[\frac{D\mathbf{v}}{Dt} - \mathbf{F} \right] \right) . \tag{3.81}$$

Special cases can be found in which both sides of (3.81) vanish, and (3.77) is satisfied in the form

$$\nabla_2 (\rho g) - f\mathbf{k} \times \frac{\partial}{\partial z} (\rho \mathbf{v}) = 0. \tag{3.82}$$

This may be re-arranged to

$$\frac{\partial}{\partial z} (\rho \mathbf{v}) = -\frac{g}{f} \mathbf{k} \times \nabla_2 \rho, \tag{3.83}$$

which is a form of the thermal wind equation. But thermal wind balance between the flow and density fields is an idealised condition which will not be precisely obeyed in reality. Even

in the simple case of a frictionless, incompressible fluid described by quasi-geostrophic (QG) dynamics we have

$$\frac{\partial}{\partial z}\left(\rho\left[\frac{D\mathbf{v}}{Dt}-\mathbf{F}\right]\right) \;\rightarrow\; \frac{\partial}{\partial z}\left(\rho_0\frac{D\mathbf{v}_g}{Dt_g}\right)=\frac{\partial}{\partial z}\left(\rho_0\left[\frac{\partial}{\partial t_g}+\mathbf{v}_g\cdot\nabla\right]\mathbf{v}_g\right), \tag{3.84}$$

and it is readily shown that the geostrophic advection term has both divergent and rotational parts, in general. [Here $\mathbf{v}_g$ is the (non-divergent) geostrophic flow in the QG model.]

All this means that calculating p^G from (3.74) applied at various levels does not ensure hydrostatic balance with the density field ρ, even if the flow is *quasi*-geostrophic. In practice, one will assume hydrostatic balance and conclude that the density structure is different from ρ. This, we believe, is one reason for the inferred temperature structure being inconsistent with the known temperature structure. (Another reason is the recognised inappropriateness of treating as balanced those rotational wind increments that are not even quasi-geostrophic, which the use of (3.71) to calculate p^G inevitably allows. Both reasons are covered by the statement that the density and temperature fields implied by (3.74) (and $p=\rho RT$) will be realistic only to the extent that thermal wind balance exists.)

Solving a 3D Poisson equation would perhaps make these ills less apparent, but it would not cure them. From the geostrophic and hydrostatic relations in the forms (3.69) and (3.75) we readily find

$$\nabla_2^2 p^G+\frac{\partial^2 p^G}{\partial z^2}=-\nabla_2\cdot(\rho f\mathbf{k}\times\mathbf{v})-g\frac{\partial\rho}{\partial z}\,. \tag{3.85}$$

However, solving this 3D Poisson equation, even subject to the condition

$$\frac{\partial p^G}{\partial z}=-\rho g \tag{3.86}$$

at the top and bottom boundaries, would not in general give a solution that obeyed equation (3.86) and

$$\nabla_2^2 p^G=-\nabla_2\cdot(\rho f\mathbf{k}\times\mathbf{v}) \tag{3.87}$$

at interior points. Indeed, the solution would in general obey neither (3.86) nor (3.87) at interior points. In some ways this might be preferable to (3.87) being satisfied everywhere and (3.86) nowhere (except at incidental special points), but the basic problem would have been diluted amongst the available spatial dimensions rather than reduced in any absolute sense. Neither would the inappropriateness of treating unbalanced rotational flow as balanced have been addressed.

4 Balance in VAR (Appendix 4)

Control of imbalance

When variational analysis (VAR) is part of a forecasting system, imbalance can be controlled either by procedures such as non-linear normal mode initialization which are external to VAR, or by internal procedures such as the introduction of a third penalty term J_c to the definition (1.1) of the total penalty J. Fisher (private communication) has argued that Bayesian probabilistic interpretation of the component terms of the total penalty J suggests that mass-wind coupling could and should be introduced through a J_c term alone, without additional external initialization. From Bayes theorem, the J_c term should quantify the probability of the atmosphere being in state $\mathbf{x}$, given our knowledge of balance.

The control of imbalance is a key issue in the design and operation of a forecasting system, but it can be considered independently of the choice of control fields. Our discussion of balance in this document is mainly in the context of that choice, in which the major concern is the identification of control fields whose forecast errors are only weakly correlated. Of course, we would require any J_c term to be expressible in terms of the chosen control fields.

Current choice of unbalanced flow control fields

At present, the sole balanced control field in our VAR system is the streamfunction, ψ, which describes the rotational, non-divergent part of the horizontal flow $\mathbf{u}$ according to a (purely kinematic) Helmholtz decomposition:

$$\mathbf{u} = \mathbf{k} \times \nabla\psi + \nabla\chi. \tag{4.88}$$

Here $\mathbf{k}$ is unit vector in the upward vertical direction, and ∇ is the horizontal gradient operator; χ is the velocity potential of the divergent, irrotational flow and is chosen as a control field. As we have noted in the main text, an undesirable feature of this scheme is that *all* the divergent flow is treated as unbalanced; it would be more satisfactory to subtract from χ a balanced contribution (related in some way to the balanced flow control field) and to choose the residual as a control field. An advantage of such a scheme, if applied to subtract balanced components also from other control fields, would be an ability to project information from moisture observations onto the horizontal momentum balance. Note that

a residual scheme of the envisaged type might retain the streamfunction ψ as balanced-flow control field, or might choose a new balanced-flow control field; various possibilities are described in later paragraphs.

Currently, the third control field is an unbalanced pressure, defined by

$$ {}^{A}P \equiv {}^{H}P - {}^{F}P. \tag{4.89}$$

Here ${}^{H}P$ is a hydrostatically-balanced pressure, and ${}^{F}P$ is a geostrophically-balanced pressure obtained by solving a linear balance equation and then applying a vertical regression procedure. The weakness of this scheme is the two-dimensionality introduced by linear balance: it compromises vertical consistency (as discussed in Appendix 3) and necessitates the regression procedure. Difficulties with the current scheme also occur when surface friction is included (S. Dance, private communication).

Work of Cullen and Wlasak

In view of the shortcomings noted in the previous paragraph, Cullen (2002b) suggests an improved scheme based on the use of potential vorticity as a control field. Wlasak (2002) has studied the scheme in some detail using a shallow water model. The central equations are the linear balance equation and the Rossby formula for potential vorticity, q:

$$\nabla \cdot (f\mathbf{k} \times \mathbf{u}) + g\nabla^2 h = 0 \tag{4.90}$$

$$\frac{\mathbf{k} \cdot (\nabla \times \mathbf{u}) + f}{h} = q. \tag{4.91}$$

Here h is the depth of the fluid, g is gravity and f is the Coriolis parameter. The horizontal flow is represented in terms of a stream function as $\mathbf{u} = \mathbf{k} \times \nabla\psi$ and is thus assumed to be non-divergent. Regarding q as a known function of position, we can consider (4.90) and (4.91) as two equations in the two unknowns ψ and h.

The control fields are defined as follows. (i) A balanced stream function ψ^b and a balanced height h^b are defined as the solutions of (4.90) and (4.91) obtained when q is computed from "real" data. (ii) An unbalanced stream function ψ^{ub} and an unbalanced height h^{ub} are defined as the solutions of (4.90) and (4.91) obtained when the left-hand side of (4.90) is evaluated from "real" data (and thus allowed to be non-zero) and q is set equal to zero in (4.91); i.e.

$$-\nabla \cdot \left(f\nabla\psi^{ub}\right) + g\nabla^2 h^{ub} = \nabla \cdot (f\mathbf{k} \times \mathbf{u}) + g\nabla^2 h \tag{4.92}$$

$$\frac{\nabla^2\psi^{ub} + f}{h^{ub}} = 0. \tag{4.93}$$

A fifth variable is velocity potential. Wlasak studies the different choices of one balanced and two unbalanced fields from this family, and examines how well each choice captures the imbalance in flows with different Burger number.

A disadvantage of this methodology is that the divergent component of the flow is treated as entirely unbalanced.

A scheme using potential vorticity and incorporating a balanced divergent wind

White (2002), section 9.4, describes the semi-geostrophic equations for shallow-water flow, and compares the accuracy of the vorticity derived from this system with that of the "standard" non-linear balance equation derived from the divergence equation. The expression for the vorticity in these different cases can be expressed in terms of a nonlinear Monge-Ampere equation arising in the asymptotic expansion of the vertical component of the vorticity to second order in the Rossby number:

$$\zeta^C \equiv f_0 + \frac{\partial v_g}{\partial x} - \frac{\partial u_g}{\partial y} + \frac{\alpha}{f_0} J\left(u_g,\, v_g\right). \tag{4.94}$$

Here f_0 is a datum value of the Coriolis parameter, and

$$J\left(u_g,\, v_g\right) = \frac{\partial u_g}{\partial x}\frac{\partial v_g}{\partial y} - \frac{\partial v_g}{\partial x}\frac{\partial u_g}{\partial y}. \tag{4.95}$$

The Monge-Ampere form of (4.94) emerges when $(u_g,\, v_g) = \mathbf{v}_g = f_0^{-1}\mathbf{k} \times \nabla\varphi$ is used to substitute for the geostrophic wind components u_g and v_g in terms of the geopotential φ ($= gh$ in shallow water theory). In (4.94), ζ^C is the vorticity defined by the balance condition, and the constant α takes different values depending on which balance condition is applied: $\alpha = 0$ corresponds to simple geostrophic balance, $\alpha = 1$ to semi-geostrophic balance, and $\alpha = -2$ to nonlinear balance. The superscript C stands for "constraint", a term having its origins in the Hamiltonian theory of balanced models described by McIntyre and Roulstone (1996, 2002).

It can be shown (McIntyre and Roulstone 1996) that $\zeta^C = f_0 + \mathbf{k} \cdot \nabla \times \mathbf{u}^C$, where

$$\mathbf{u}^C = \mathbf{u}_g - \frac{\alpha}{2f_0}\mathbf{k} \times \left[\left(\mathbf{u}_g \cdot \nabla\right)\mathbf{u}_g\right]. \tag{4.96}$$

Typically $\nabla \cdot \mathbf{u}^C \neq 0$, i.e. $\mathbf{u}^C$ has a divergent part.

In the control field transforms, we could use $\mathbf{u}^C$ instead of $\mathbf{k} \times \nabla\psi$. (i) Increments to a balanced mass field would be obtained by linearizing the potential vorticity

$$q = \frac{\left(f + \zeta^C\right)}{\varphi} \tag{4.97}$$

using

$$\varphi^b = \overline{\varphi} + \delta\varphi^b \tag{4.98}$$

in (4.94). The resulting variable-coefficient Poisson equation for $\delta\varphi^b$ would then be solved given δq from model data (i.e. $\overline{\varphi}$, $\delta\varphi$ and $\delta\zeta = \mathbf{k} \cdot \nabla \times \delta\mathbf{u}$). (ii) $\delta\mathbf{u}^C$ would then be found using (4.95) and (4.96). (iii) The unbalanced divergence, $\nabla^2\delta\chi^S$, and unbalanced vorticity, $\nabla^2\delta\psi^S$, would be defined in terms of the "velocity split" $\delta\mathbf{u}^S = \delta\mathbf{u} - \delta\mathbf{u}^C$ of McIntyre and Roulstone by

$$\nabla^2\delta\chi^S = \nabla \cdot \delta\mathbf{u}^S, \quad \nabla^2\delta\psi^S = \mathbf{k} \cdot \nabla \times \delta\mathbf{u}^S. \tag{4.99}$$

The vector field $\delta\mathbf{u}^S = \delta\mathbf{u} - \delta\mathbf{u}^C$ can be thought of as a generalization of ageostrophic motion with respect to the vector field $\delta\mathbf{u}^C$. (iii) The unbalanced mass field, $\delta\varphi^{ub}$ would be defined as a solution of the linearised potential vorticity equation when $\delta q = 0$.

In this scheme, the U_p transform would be defined by the following steps:

(a) Calculate $\delta\mathbf{u}^C$ from $\delta\varphi^b$ (using (4.95) and (4.96); differentiation)

(b) Calculate $\delta\mathbf{u}^S$ from $\delta\psi^S$ and $\delta\chi^S$ (using $\delta\mathbf{u}^S = \mathbf{k} \times \nabla\delta\psi^S + \nabla\delta\chi^S$; differentiation)

(c) Form $\delta\mathbf{u} = \delta\mathbf{u}^C + \delta\mathbf{u}^S$

(d) Form $\delta\varphi = \delta\varphi^b + \delta\varphi^{ub}$

Note that $\delta\mathbf{u}^C$ could be used to calculate geostrophically-balanced increments to vertical motion via Richardson's equation. This might be important in projecting information from the assimilation of moisture onto balanced dynamical modes.

A disadvantage of the proposed scheme is that it is couched in the usual f-plane terms of semi-geostrophic theory; it isn't clear how variable f should be handled. Another disadvantage is that the balanced divergence $\nabla \cdot \mathbf{u}^C$ that the scheme allows does not transparently correspond to the divergence implied by a suitable form of the omega equation.

The slow equations (Lynch 1989)

A scheme that permits a balanced component of the divergence, but avoids the difficulties of Coriolis parameter variation that bedevil asymptotic expansions based on geostrophy, can be formulated from P. Lynch's *Slow Equations*. This scheme also more transparently relates divergence to the preservation of geostrophic balance in the time evolution. Following Lynch, the shallow water equations can be written in terms of vorticity ζ and divergence D as

$$\zeta_t + fD = -N^\zeta \tag{4.100}$$

$$D_t - f\zeta + \nabla^2\varphi = -N^D \tag{4.101}$$

$$\varphi_t + \overline{\varphi}D = -N^\varphi. \tag{4.102}$$

Here the subscript t denotes $\partial/\partial t$, and N^ζ, N^D, N^φ represent the nonlinear terms:

$$N^\zeta \equiv \mathbf{u}\cdot\nabla\zeta + \zeta D + \beta_y v + \beta_x u \tag{4.103}$$

$$N^D \equiv \mathbf{u}\cdot\nabla D + D^2 - 2J(u,v) + \beta_y u - \beta_x v \tag{4.104}$$

$$N^\varphi \equiv \mathbf{u}\cdot\nabla\varphi + (\varphi - \overline{\varphi})\, D \tag{4.105}$$

[Cartesian geometry is assumed, but the x axis is not necessarily aligned west-east: the terms β_x and β_y allow for variation of the Coriolis parameter in both the x and the y directions.]

The tendencies of the divergence and of the geostrophic imbalance ($\epsilon \equiv \nabla^2\varphi - f\zeta$) project onto gravity modes. To define balance we set these tendencies to zero:

$$\nabla^2\varphi - f\zeta = -N^D \tag{4.106}$$

$$\left[\nabla^2 - \frac{f^2}{\overline{\varphi}}\right](\overline{\varphi}D) = fN^\zeta - \nabla^2 N^\varphi. \tag{4.107}$$

The (conserved) potential vorticity is

$$q = \frac{f+\zeta}{\varphi}. \tag{4.108}$$

We use (4.108) (with $q \neq 0$), (4.106) and (4.107) to define balanced mass and wind fields φ^b, ψ^b , χ^b . Imbalance is defined by $q = 0$, and we use the divergence tendency, D_t, and the tendency of the geostrophic imbalance, ϵ_t, to define unbalanced mass and wind fields φ^{ub}, ψ^{ub} , χ^{ub}. The scheme may be summarised as follows:

1. To define balance, calculate q from model data and apply (4.106) and (4.107).

2. To define imbalance, calculate D_t and ϵ_t from model data (using suitable modifications of (4.106) and (4.107), which as they stand assume $D_t = \epsilon_t = 0$) and apply $q = 0$.

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