On the Completeness of Multi-Variate Optimum Interpolation for Large-Scale Meteorological Analysis

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ABSTRACT

The Baer-Tribbia nonlinear modal initialization method implies that large-scale meteorological analyses should focus on analysis of slow mode fields. An idealized multi-variate optimum interpolation analysis is shown to produce grid point results that contain only slow modes. Variational analysis with a slow mode constraint is therefore unnecessary.

1. The consequences for analysis of nonlinear modal initialization

Baer and Tribbia (1977) have shown how initial conditions for a large-scale numerical model can be determined so that there is no "noise" in a forecast from this initial state. Their procedure is related to the Machenhauer (1976, 1977) method, but is based on a formal expansion using the smallness of the ratio between Rossby mode frequencies and gravity mode frequencies. These modes are the solutions to the linearized equations of the forecast model for perturbations on a resting basic state. Using a simple f-plane Boussinesq model, Leith (1980) has shown that the initial steps of the Baer-Tribbia method (*but not the Machenhauer method*) are equivalent, in extratropical latitudes, to quasi-geostrophic computations of divergence and non-geostrophic vorticity. (This difference occurs because the Baer-Tribbia method starts by discarding all fast modes, while the Machenhauer method does not.)

Leith has also provided a convenient graphical description of initialization with his concept of the *slow manifold.* In Fig. 1, we consider the abscissa as representing an additive measure of squared amplitudes of the slow modes contained in a complete three-dimensional meteorological field, and the ordinate as the corresponding measure of the fast mode components. (*Slow* and *fast* would normally be identical with *Rossby* and *gravity*, but are preferable names in that they recognize the freedom to choose the frequency separation criterion for best results. Some authors use the adjective "slow" only with respect to *states* on the slow manifold. *Slow modes*, as used in this paper, refer only, as stated here, to the modes of the rest basic state that are held fixed in nonlinear initialization.) The collection of all balanced states can be indicated by a schematic "curve" in this highly compressed diagram. Leith has given the name "slow manifold" to this collection of balanced states. This is because the Baer-Tribbia formalism assumes that in a balanced state, the fast mode components are not arbitrary, but are determined (i.e. forced) by the nonlinear interaction of all the slow modes in that state. The atmosphere and model are assumed to be located on this manifold at all instants.

The Baer-Tribbia initialization process begins with a field containing only slow modes, such as would be obtained from a general analysis by subtracting all fast modes. The nonlinear interactions of the slow modes produce tendencies ($\partial u/\partial t$, etc.) that have fast mode components. In the first Baer approximation, these components are to be cancelled by the linear tendencies of the unknown fast modes so that the total tendency of fast modes vanishes to this order of approximation. This determines the first iterative solution for the fast mode amplitudes.

The process for further iterations is well-defined, and the only mathematical problems are those of convergence of the iterations and the increasing computation associated with each iteration (Ballish, 1980). A meteorological problem also arises in that certain slow motions of importance in low latitudes involve a balance between strong release of latent heat and the vertical motions associated with gravity wave modes. Temperton (1980, p. 183) has suggested that the slow manifold must therefore be displaced upward in Leith's diagram as a "non-adiabatic" slow manifold to recognize this exception to the basic assumption underlying the Baer process.

This exception will require special consideration (for example, specification of the temperature tendency from latent heat as a known quantity) and in this paper I assume that a satisfactory treatment of this can be achieved. It is then possible to recognize the dependent character of the fast mode components

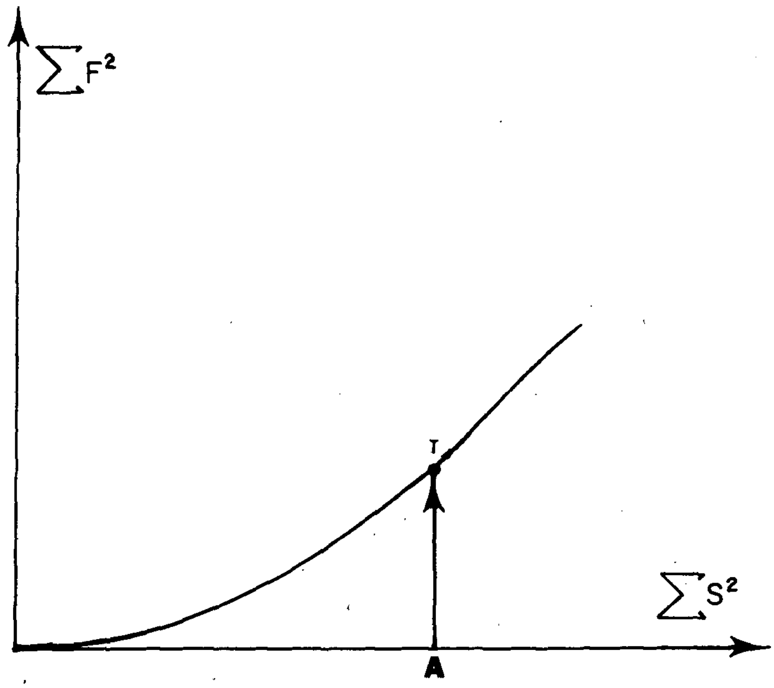

FIG. 1. The slow manifold diagram of Leith. Point A represents a slow mode analysis. The arrow AT denotes the Baer-Tribbia nonlinear modal initialization process.

in an initial field and draw the following logical consequences of the Baer initialization process:

I) *The purpose of large-scale meteorological analysis is to obtain the most accurate possible depiction of the slow mode fields.*

Two further consequences result immediately:

II) *Observations used in this slow mode analysis must be corrected for the fast mode components that they contain.*

III) *Any statistical-dynamical guidance used in analyzing slow mode fields must be based on the kinematic properties of only slow mode fields, not on the properties of complete fields.*

In a recent paper, Phillips (1981) showed how procedure II can be implemented, and the importance of doing so with respect to obtaining maximum accuracy of the analysis in data-rich areas. This demonstration was couched in terms of the strict constraint variational analysis method introduced by Y. Sasaki (1958). As a useful technique, this analysis method is far removed from operational practice, however, because it is designed to use input data located only at grid points, and becomes complex as soon as one begins to allow for the existence of correlations between the input grid-point data errors (see Section 4).

The remainder of this paper proves a "theorem" that obviates the use of a variational analysis to enforce the constraint that the analysis is to result in an analysis of slow modes only. The theorem can be stated as follows:

A multivariate optimum interpolation analysis will result in grid-point values containing only slow modes if three conditions are met:

1) It is given a first guess containing only slow modes.

2) The first guess error covariances that it uses are for slow mode errors only, and are specified by a power spectrum of slow mode error.

3) All observations are used in the analysis for each grid-point variable.

The theorem does not address the accuracy of the "observations" with respect to statement II above, this point having been addressed in the previous paper. The ideas of optimum interpolation (O/I) that were originally formulated by Gandin (1963) and Eliassen (1954), and implemented most recently by Lorenc (1981), are therefore in principle capable of responding completely to the theoretically based needs of modern large-scale meteorological analysis.[1]

[1] A preliminary version of this paper has been written as Office Note 250 of the National Meteorological Center. It contains a detailed analysis of the modes in a one-dimensional space.

2. Optimum interpolation

Let K denote the number of grid-point variables in a complete three-dimensional analysis of the dynamical variables. In a grid array composed of K_h horizontally-spaced locations and K_v levels in the vertical, K will equal K_h $(3K_v + 1)$, representing two velocity components and a temperature at each point, together with a surface pressure field. These K numbers will be represented as a vector Y_k, $k = 1, K$. Y_k(an) will denote the result of an optimum interpolation, and Y_k(fg) will denote the slow mode first guess field that is to be updated with observations to produce Y_k(an).

Let Z_p, $p = 1, P$ denote the collection of observations. The O/I analysis (Lorenc, 1981) is calculated as a correction to Y_k(fg):

$$Y_k(\text{an}) = Y_k(\text{fg}) + \sum_{p=1}^{P} \alpha_{kp}[Z_p - Y_p(\text{fg})], \quad (2.1)$$

where Y_p(fg) is the first guess variable corresponding in type and location to the observation Z_p. (Since observations need not be at grid points, special consideration must be given to defining a first guess value at an observation point. This is done in Section 3.)

In this paper we assume that conditions 1–3 listed in Section 1 are obeyed. Y_k(fg) and Y_p(fg) therefore contain only slow modes, and the observations Z_p have been "corrected" by having a fast mode field subtracted from them as described in Phillips (1981). Note that in (2.1) it is assumed that all observations are used to update each analyzed value.

The coefficients α_{kp} in (2.1) are determined by minimizing the expected squared error in each Y_k(an). This results in K sets of P equations each. They have the form ($p, q = 1, P$):

$$\sum_{p=1}^{P} \alpha_{kp}\overline{(z_p - y_p)(z_q - y_q)} = \overline{y_k y_q} - \overline{y_k z_q}\,, \quad (2.2)$$

where

$$z_p = \text{error of observation } p, \quad (2.3a)$$

$$y_p = \text{first guess error at } p. \quad (2.3b)$$

(Recall that subscripts denote not only spatial position but also variable type.)

Let $\mathbf{O}_{pq}$ denote the inverse of the symmetric error covariance matrix $\overline{(z_p - y_p)(z_q - y_q)}$:

$$\mathbf{O}_{pq} = (\overline{z_p z_q} + \overline{y_p y_q} - \overline{z_p y_q} - \overline{z_q y_p})^{-1}. \quad (2.4)$$

The O/I analysis formula is then

$$Y_k(\text{an}) = Y_k(\text{fg}) + \sum_{p=1}^{P} [Z_p - Y_p(\text{fg})] \sum_{q=1}^{P} \mathbf{O}_{pq}(\overline{y_k y_q} - \overline{y_k z_q}). \quad (2.5)$$

In current operational practice it is customary to ignore correlation of first guess and observational errors. This is certainly not justified if the first guess comes from an assimilation system having frequent updates and observation errors that are not completely random. We therefore develop our mathematical analysis so that this effect can be considered.

3. Modes and first guess errors

The analysis (2.5) requires statistical estimates of first guess error at grid points and at observation points. To accomplish this we generalize the grid point vector notation Y_k so as to represent a specialization of continuous fields $Y(\mathbf{x})$ by evaluation of the latter at the points $\mathbf{x}_k$. Thus,

$$Y_k \equiv Y(\mathbf{x}_k). \quad (3.1)$$

The symbol $\mathbf{x}$ by itself denotes both the choice of variable (velocity, temperature, surface pressure) and a location in the atmosphere. The subscript k will specialize the location of the variable to a grid point. The subscript p or q will specialize the location of the variable to an observation point.

We postulate the existence of a complete set of discrete continuous orthogonal eigenfunctions $\phi_l(\mathbf{x})$, $l = 1, K$, which, when evaluated at the grid points are sufficient to represent any $Y(\mathbf{x}_k)$:

$$Y(\mathbf{x}_k) = \sum_{l=1}^{K} \Phi_l \phi_l(\mathbf{x}_k). \quad (3.2)$$

At this point, $Y(\mathbf{x}_k)$ represents an arbitrary field, not just a field of slow modes.

For simplicity we can assume the orthonormalization of ϕ_l to be defined with respect to a simple grid-point sum:

$$\sum_{k=1}^{K} \phi_l(\mathbf{x}_k)\phi_m(\mathbf{x}_k) = \begin{cases} 0 & \text{for} \quad l \neq m, \\ 1 & \text{for} \quad l = m. \end{cases} \quad (3.3)$$

Then the expansion coefficients Φ_l are given by

$$\Phi_l = \sum_{k=1}^{K} Y(\mathbf{x}_k)\phi_l(\mathbf{x}_k). \quad (3.4)$$

The general distribution at all $\mathbf{x}$ is defined by the continuous eigenfunctions, using the same Φ_l:

$$Y(\mathbf{x}) = \sum_{l=1}^{K} \Phi_l \phi_l(\mathbf{x}). \quad (3.5)$$

This convention is similar to the horizontal relations used in spherical harmonic transform forecast models.[2]

[2] In the vertical direction the continuous variation must be obtained either by interpolation of the finite level eigenvectors used in obtaining normal modes of a forecast model, or the latter must be derived from a Galerkin representation in the vertical, with special attention to the upper boundary condition.

We now formally separate the K eigenvectors into a set of L "slow modes"

$$s_l(\mathbf{x}) = \phi_l(\mathbf{x}), \quad l = 1, L \tag{3.6}$$

and a separate set of $K - L$ "fast modes"

$$f_l(\mathbf{x}) = \phi_{l+L}(\mathbf{x}), \quad l = 1, K - L. \tag{3.7}$$

Let S_l, F_l denote the amplitudes of these modes in a field. A field of slow mode errors $y(\mathbf{x})$ is then specified by

$$y(\mathbf{x}) = \sum_{l=1}^{L} \delta S_l s_l(\mathbf{x}), \tag{3.8}$$

if δS_l is the error in slow mode amplitude S_l. We can now express the slow mode first guess error covariance $\overline{y_k y_q}$ as

$$\overline{y_k y_q} = \sum_{l=1}^{L} s_l(\mathbf{x}_k) \sum_{m=1}^{L} (\overline{\delta S_l \delta S_m}) s_m(\mathbf{x}_q). \tag{3.9}$$

The $\overline{y_k y_q}$ covariance term in (2.5) can be written formally as[3]

$$-\overline{y_k z_q} = -\sum_{l=1}^{L} [\overline{z_l \delta S_l}] s_l(\mathbf{x}_k). \tag{3.10}$$

The optimum interpolation analysis equation (2.5) can now be written as

$$Y_k(\text{an}) = Y_k(\text{fg}) + \sum_{p=1}^{P} [Z_p - Y_p(\text{fg})] \sum_{q=1}^{P} \mathbf{O}_{pq} \sum_{l=1}^{L} T_l(\mathbf{x}_q) s_l(\mathbf{x}_k), \tag{3.11}$$

where $T_l(\mathbf{x}_q)$ incorporates the appropriate parts of (3.9) and (3.10). The projection of $Y_k(\text{an})$ onto the fast mode eigenvectors $\mathbf{f}(\mathbf{x}_k)$ is quickly seen to be zero. First, $Y_k(\text{fg})$ by definition contains only slow modes. Second, the projection operator $\sum_k \mathbf{f}(\mathbf{x}_k)$ can be brought inside the p, q and P sums in (3.11). The orthogonality of $\mathbf{f}(\mathbf{x}_k)$ and $s_l(\mathbf{x}_k)$ then produces a zero result.

This proof that the multivariate O/I grid point analysis contains only slow modes is seen to rest upon three conditions: a) the first guess $Y_k(\text{fg})$ contains only slow modes, b) the first guess errors y are for slow modes only, with their covariance specified as a continuous function of space by the spectral representation (3.9), and c) all observations are used in obtaining each Y_k. (The third of these is necessary to allow the k-sum projection operator to be moved inward past the p and q sums. If the latter sums differed for different Y_k, this transposition would not be permissable.)

Finally in this section, it should be noted that the eigenfunctions s_l, f_l need only have the formal properties contained in (3.2)–(3.6). Those statements have no dynamic content; the use of adjectives "slow" and "fast" is only relevant with respect to the choices made in the Baer-Tribbia initialization technique.

[3] The observation error can be expressed as a random component plus a term proportional to the true field $Z_q(\text{tr})$. The latter can in turn be expressed as the first guess $Y_q(\text{fg})$ minus the first guess error y_q. The principal information needed is the correlation $\overline{Y_q(\text{fg}) y_q}$.

4. Variational analysis

Variational analysis with a strict constraint was introduced into meteorology by Sasaki (1958). This allows two different fields to be improved in their accuracy by mutual adjustment. Daley (1978) used it to explore the possibility of combining the Machenhauer initialization procedure with analysis of grid point data. Phillips (1981) also used variational analysis, to demonstrate the increased accuracy achievable by purposely performing analyses of the slow modes alone.

These two studies, and other references to variational analysis in the literature, have assumed that input data are available on grid points. Since optimum interpolation efficiently interpolates data to grid points, it might seem that a logical procedure would be simply to follow the optimum interpolation process with a variational analysis (e.g., Phillips, 1981, Section 6). However, the previous three sections have demonstrated the completeness of the idealized multivariate optimum interpolation in that linear constraints can be satisfied precisely in the process of interpolating to grid points.

The result is that variational analysis is no longer needed to improve the accuracy of analyzed fields by the use of kinematic constraints. The following brief analysis may be useful by establishing this point in more detail (and also by suggesting the proper way to treat correlated errors in variational analysis).

The essence of the Sasaki procedure is to use input values X_j^0 to obtain analyzed-values X_j that will minimize a positive definite functional

$$\text{SAS} = \sum_{j=1}^{J} W_j (X_j - X_j^0)^2, \quad W_j > 0, \tag{4.1}$$

and also obey M linear constraints

$$\sum_{j=1}^{J} R_{mj} X_j = 0, \quad m = 1, M. \tag{4.2}$$

If the errors δX_j^0 in the input data are independent, so that $\overline{\delta X_l^0 \delta X_j^0} = 0$ when $l \neq j$, the optimum choice for W_j in (4.1) is the reciprocal of $\overline{(\delta X_j^0)^2}$:

$$W_j(\text{opt}) = 1/\overline{(\delta X_j^0)^2}. \tag{4.3}$$

[This also allows the expression on the right side of (4.1) to be given a probability interpretation.]

In our case the input data X_j^0 is given by $Y_j(\text{an})$, as defined in (3.9). The errors δY_j in $Y_j(\text{an})$ will be correlated, however, so that (4.3) does not immediately apply. Instead it is necessary to perform the preliminary step of projecting $Y_j(\text{an})$ onto the orthonormal eigenvectors ϵ_{jk} of the error covariance matrix $\overline{\delta Y_j \delta Y_k}$:

$$w_j^0 = \sum_{k=1}^{K} \epsilon_{jk} Y_k(\text{an}). \qquad (4.4)$$

$\overline{\delta w_j^0 \delta w_i^0}$ is now zero if $j \neq i$. $\overline{(\delta w_j^0)^2}$ is equal to λ_j, the nonnegative eigenvalue associated with ϵ_{jk}. Its reciprocal is the desired weight W for (4.1):

$$\text{SAS} = \sum_{j=1}^{K} (w_j - w_j^0)^2/\lambda_j\,, \qquad (4.5)$$

where w_j is the output of the variational process.

Although the input data vector $Y_k(\text{an})$ is of length K, it has only L degrees of freedom since it contains no fast mode components. This means that there are $K - L$ linear combinations of $Y_k(\text{an})$ for which

$$\sum_{k=1}^{K} \beta_{kn} \delta Y_k = 0, \quad n = 1, K - L. \qquad (4.6)$$

Because of this, there will be $K - L$ error covariance eigenvectors that have zero eigenvalues λ_j. In (4.5) this means that the corresponding values of $w_j - w_j^0$ must be zero in order to minimize the Sasaki functional. Thus (4.5) is in effect replaced by the reduced sum

$$\text{SAS} = \sum_{j=1}^{L} (w_j - w_j^0)^2/\lambda_j\,, \quad \lambda_j > 0. \qquad (4.7)$$

The constraint that we wish to impose is still the constraint that the adjusted field consist only of slow modes. Each of the L output w's of the variational analysis must therefore be expressible in the form

$$w_j = \sum_{k=1}^{K} \epsilon_{jk} \sum_{l=1}^{L} S_l s_l(\mathbf{x}_k) = \sum_{l=1}^{L} U_{jl} S_l\,. \qquad (4.8)$$

But since $Y_k(\text{an})$ contains only slow modes, w_j^0 in (4.4) can also be written in the same form:

$$w_j^0 = \sum_{l=1}^{L} U_{jl} S_l^0. \qquad (4.9)$$

The Sasaki functional becomes

$$\sum_{j=1}^{L} \frac{1}{\lambda_j} [\sum_{l=1}^{L} U_{jl}(S_l - S_l^0)]^2 = \text{minimum}.$$

Since all constraints have been applied, the solution that minimizes this is simply $S_l = S_l^0$. Thus, the application of the Sasaki strict constraint variational analysis to the output fields of an idealized optimum interpolation analysis will produce no change.

5. Relation to current practice

To what extent do current optimum interpolation analyses satisfy the three consequences and the three conditions described in section 1? As a "state-of-the-art" operational system I will refer to the most recently described system, that of the European Centre for Medium Range Weather Forecasts (ECMWF), which is described by Lorenc (1981). The analysis equation (2.5) is useful to refer to in arriving at the following comments:

$$Y_k(\text{an}) = Y_k(\text{fg}) + \sum_{p=1}^{P} [Z_p - Y_p(\text{fg})] \sum_{q=1}^{P} \mathbf{O}_{pq}(\overline{y_k y_q} - \overline{y_k z_q}). \qquad (5.1)$$

1) In this paper, the term $[Z_p - Y_p(\text{fg})]$ in (5.1) represents the difference between an observation $Z_p(\text{total})$ minus a fast mode estimate, and the slow mode first guess $Y_p(\text{fg})$. If the fast mode estimate of Z_p is that contained in the first guess, this result is equal to $Z_p(\text{total})$ minus the total first guess. This is then equal to the residual used in operational practice.[4]

2) In this paper $Y_k(\text{fg})$ on the right side of (5.1) is the slow mode part of the first guess, whereas in operational practice, the full first guess is added to the correction sum. $Y_k(\text{an})$ then contains all fast modes in the first guess. However, if the nonlinear initialization that is used operationally after the analysis is the Baer-Tribbia procedure, the first step is to discard any fast modes in $Y_k(\text{an})$. The fast mode content of $Y_k(\text{fg})$ is then irrelevant and this condition of this paper is satisfied. At the time of writing, ECMWF uses a Machenhauer initialization, however, in which forecast fast modes are not discarded at the start of initialization.

3) An obvious difference is that (5.1) requires the use of all observations for updating each analyzed value. If interpreted literally, this is impractical. Intelligent compromises are certainly possible, at least with the fastest computers now available. For example, at ECMWF the analysis does satisfy this completeness requirement within each analysis volume.

4) $\mathbf{O}_{pq}$ and $\overline{y_k y_q}$ in (5.1) are defined in this paper by errors in slow modes in the spectrally based equation (3.9). In practice these are modeled by assuming a horizontally translatable plan form or shape with a spatially variable amplitude. Lorenc (1981, p. 707) has discussed some of the mathematical "constraints"

[4] If the data are very accurate compared to the first guess, the fast mode component of the first guess may not provide a satisfactory correction to $Z_p(\text{total})$ to give $Z_p(\text{slow mode})$. In this case it may be necessary to re-examine this correction using the fast modes that the Baer-Tribbia procedure will derive from $Y_k(\text{an})$ (Phillips, 1981).

that must be considered in using this type of correlation model. Although these considerations would be largely unnecessary if (3.9) were used, this is not a major deviation from the point of view of this paper. In extratropical latitudes, the slow modes s_l are highly geostrophic and non-divergent. This constraint between mass and wind fields is satisfied by the geostrophic covariance model used at ECMWF and other centers. In low latitudes, however, the slow modes are much less geostrophic and are no longer highly non-divergent. We therefore cannot expect the ECMWF scheme (Lorenc, 1981, pp. 706–7) to reproduce the results of (3.9) in these regions.

5) The horizontal scale in the commonly used Gaussian function for height–height forecast error covariance is based on experimental data consisting of total errors in forecast height. A different scale (and possibly a more interesting horizontal plan form) might result if these computations were redone using only slow mode forecast height errors. However, a more fundamental improvement might be achieved if the local scale and the local amplitude of the error covariance model were both predicted as a function of past data and the meteorological background. The formula (3.9) may be helpful in this regard, through its prescription of a general error covariance model with ideal properties, that practical formulations should approximate. Ghil *et al.* (1981) have drawn attention to the relation of Kalman filtering to the careful prediction of forecast error covariances.

In summary, the above comparison of a state-of-the-art operational system with the assumptions and conclusions of this paper does not result in fundamental disagreements that are irreconcilable. Even the basic premise of this paper—that only slow modes are to be analyzed—can be considered to have been unconsciously recognized (*albeit inconsistently*) in the development of optimum interpolation techniques. The differences are to some extent matters of degree, which can be corrected with experience if the philosophy of this paper is accepted. This should also enable attention to be directed to the development of practical methods of calculating the first guess error covariances accurately as a function of time and space in an assimilation system.

The inconsistencies in current analysis practice can be confusing, however. For example, Williamson *et al.* (1981) have published an empirical study of the mass–velocity balance resulting from optimum interpolation analysis. In speaking of sources of imbalance, they conclude (p. 2372) "we find multivariate optimal interpolation to be the most important as it can introduce systematic imbalances which result in relatively large changes when initialization is performed." This conclusion appears opposite to that reached in this paper. It results from the attempt by these authors (in common with others) to directly analyze complete fields instead of analyzing slow modes only. According to the view presented in Section 1 of this paper, one must expect initialization to change analyzed fields because initialization is needed to add the balancing fast modes. A correct analysis of slow modes will result in a data fit that is improved upon Baer-Tribbia initialization. This final step of initialization must be anticipated in designing the preceding analysis steps.

Acknowledgments. This study was originally developed to test the view of A. Hollingsworth and A. Lorenc that variational analysis should not be necessary as a follow-on to a univariate optimum interpolation analysis. The final form was sharpened through discussion with P. Long, D. Parrish and R. McPherson.

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