Interpretations of the total energy and rotational energy norms applied to determination of singular vectors

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SUMMARY

The interpretation of the commonly-used energy norm is examined in the context of a simple vertically-discrete model. The norm is shown to include expressions for kinetic and available potential energy in addition to an expression for a portion of unavailable potential energy. Another norm is then introduced that only includes the rotational-mode contribution to these. The characterization of the two norms in terms of corresponding covariance functions is shown to be quite different, with that for the latter norm looking more like prior error statistics used in synoptic-scale data assimilation. The leading singular vectors are determined for both norms. Those computed for the new norm have slower associated growth. Their corresponding structures are similar at the initial time, however, with some notable differences, but after 24 hours their shapes are almost identical. The new norm has advantages over the old norm for some applications; e.g. for effectively filtering ageostrophic, convectively-driven singular vectors and for being more consistent with a spatially and dynamically correlated error norm.

KEYWORDS: Adjoint models  Singular vectors

1. INTRODUCTION

As used in numerical weather prediction or dynamic meteorological contexts, singular vectors (SVs) are perturbation structures that grow optimally over a short period of time in a linearized model (Farrell 1988; Buizza et al. 1993). Distinct vectors can be ordered by their growth rates and are mutually orthogonal. Both the growth rates and orthogonality are defined with respect to some norm and, indeed, the SVs themselves are norm-specific, except when the forecast period is very long (Legras and Vautard 1996; Reynolds and Errico 1999).

The most common norm used to measure and constrain perturbation sizes for computing singular vectors in the context of a primitive-equation model is the ‘total energy’ norm, or E norm (Buizza et al. 1993; Ehrendorfer and Errico 1995; Palmer et al. 1998; Ehrendorfer et al. 1999). It is based on an invariant of the primitive equations when linearized about a simple reference state (Talagrand 1981; see also Lorenz 1960). It has been interpreted as the sum of kinetic energy (KE) plus an expression for available potential energy (APE), both per unit mass (Ehrendorfer and Errico 1995).

APE is defined by Lorenz (1955) as the maximum energy available for conversion to KE through an adiabatic re-distribution of mass in the atmosphere. The remaining PE is termed unavailable PE (UPE); e.g. the atmosphere’s full gravitational PE cannot be converted into KE unless the atmosphere could entirely collapse. In this report, the E norm will be shown to include some UPE in the context of a discretized form of the linearized equations used to derive the norm.

A norm determined by the $f$-plane analogue of the rotational mode subset of Hough functions, termed an R norm, was introduced by Ehrendorfer and Errico (1995). That norm was primarily intended to remove explicit consideration of inertial-gravity waves from the E norm, but secondly to resemble a metric with weights determined by an inverse analysis error-covariance estimate and to reduce the size of the model space requiring explicit consideration. The model used by Ehrendorfer and Errico (1995) had an energetically inconsistent vertical discretization that disallowed defining an R norm.

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consistent with the $E$ norm. Since then, Ehrendorfer et al. (1999) have used a revised, energetically consistent model to determine SVs in the context of a moist model using an $E$ norm, for which a corresponding $R$ norm can be derived.

This paper begins by decomposing the $E$ norm into components of KE, $APE$, and $UPE$ in the context of a simple discretized model. Then a new $R$ norm is derived as the contribution to the $E$ norm by the analogue of the rotational modes on an $f$-plane. Also, a spectrally filtered version of the $R$ norm is derived. The interpretations of the $E$ and $R$ norms in terms of equivalent error covariances are described. Leading SVs determined using all three norms applied to the same model and case are then compared. Also compared are SVs determined using a modified $E$ norm that excludes $UPE$.

The $E$ norm and $R$ norm are described in sections 2 and 3, respectively. The covariance interpretation of the norms is presented in section 4. The full-physical limited-area model and case are described in section 5. Results using dry and moist linearized models are described in sections 6 and 7, respectively. Suggestions of when the truncated $R$ norm may be appropriate are offered in section 8 along with some conclusions.

2. $E$-NORM DERIVATION

The $E$ norm is typically motivated by referencing Talagrand (1981) who shows that, when linearized about an isothermal, resting atmosphere with horizontally invariant surface pressure and topography, the adiabatic primitive equations conserve an integral of a quadratic function of perturbations of wind components, temperature, and surface pressure. The analogue for a vertically discretized, periodic $f$-plane model is described in this section. The model described here, however, is not the numerical weather predicition type of model to which the norm will be applied in following sections. Neither is the state about which linearizations are performed in applications as simple as the one considered in this section. In more realistic applications, however, the simple linearized model can be useful for characterizing fields, as demonstrated by its use in nonlinear normal-mode initialization (Errico 1989).

The model considered in this section is defined for a rectangular domain with horizontal coordinates $x$ and $y$ and vertical coordinate $\sigma = p/p_s$, where $p$ is the pressure at some height and $p_s$ its corresponding surface value. No moisture or diabatic physics is considered. The boundary conditions at both $\sigma = 0$ and $\sigma = 1$ are specified as $d\sigma/dt = 0$, where $t$ is time. All fields explicitly represented below are defined on an identical set of $K\sigma$-levels, with the fields represented as a vector (indicated by bold face) at each $x$, $y$ location.

The temperature, $T$, and surface pressure about which the linearization has been performed are $T_r$ and $p_{sr}$, respectively. Perturbations from the reference state are denoted by primes. Since $p_s$ appears explicitly only as its natural logarithm, its perturbations are expressed in terms of perturbations of $\Pi = \ln(p_s/p_{sr})$.

Prognostic equations for perturbation wind components in the $x$ and $y$ directions, $T'$, and $\Pi'$ are respectively

\[ \frac{\partial u'}{\partial t} = f v' - \frac{\partial h'}{\partial x}, \]  
\[ \frac{\partial v'}{\partial t} = -f u' - \frac{\partial h'}{\partial y}, \]  
\[ \frac{\partial T'}{\partial t} = S d', \]  

(2.1)  
(2.2)  
(2.3)
\[
\frac{\partial \Pi'}{\partial t} = c^T d',
\]  

(2.4)

where \( S \) and \( c \) are matrix operators, \( d \) and \( h \) are the respective vectors whose elements are the local wind divergence and equivalent geopotential on \( \sigma \)-surfaces, \( f \) is the Coriolis parameter, and superscript \( T \) indicates a matrix (or vector) transpose. The diagnostic equations are

\[
d' = \frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y},
\]  

(2.5)

\[
h' = BT' + b\Pi',
\]  

(2.6)

where \( B \) and \( b \) are described next.

The \( K \times K \) matrices \( S \) and \( B \) are the finite-difference analogues of the respective operators

\[
-R_d T_r \int_0^\sigma \left( \frac{\partial}{\partial \sigma} \right) d\sigma',
\]

\[
R_d \int_0^1 \left( \frac{\partial}{\partial \ln(\sigma')} \right) d\ln(\sigma'),
\]

where \( R_d \) here is the gas constant for dry air, \( c_p \) is the specific heat of dry air at constant pressure, \( \sigma' \) indicates the variable \( \sigma \) used for integrations, and \(-1/p_{st}\) times the first operator applied to \( d' \) is an expression for \( \omega' = dp'/dt \). The \( K \times 1 \) matrix \( c \) is the finite-difference analogue of the operator \(-\int_0^\sigma \left( \frac{\partial}{\partial \sigma} \right) d\sigma\) and \( b \) is the vector whose \( K \) components are each \( R_d T_r \). These last two operators are therefore related by

\[
Db = R_d T_r c,
\]  

(2.7)

where \( D \) is the diagonal matrix whose components \( d_{k,k} \) are corresponding values of \( \sigma \)-layer thicknesses \( (\Delta \sigma)_k \). Conservation of total KE plus PE in a vertical finite-difference form of a primitive-equation model requires that (Hack et al. 1993)

\[
B^T D = \frac{c_p}{T_r} DS.
\]  

(2.8)

Examples of the operators \( B \) and \( c \) appear in an appendix.

From (2.3), (2.4) and (2.6),

\[
\frac{\partial h'}{\partial t} = H d',
\]  

(2.9)

where

\[
H = BS + bc^T.
\]  

(2.10)

For further details of derivation of these equations see Errico (1989).

For an energetically consistent vertical finite-difference scheme

\[
E = \frac{1}{2A} \int_X \int_Y \left( u'^T D u' + v'^T D v' + \frac{c_p}{T_r} T'^T DT' + R_d T_r \Pi'^2 \right) dy \ dx
\]  

(2.11)

is conserved by (2.1)–(2.6) with the prescribed boundary conditions on \( d\sigma/dt \) when the integrals are determined over the entire sub-domain over which the fields are assumed
periodic, and \( A \) is the area of that sub-domain. This \( E \) may be interpreted as an area averaged, energy per unit mass: the sum of the \( u' \) and \( v' \) contributions yielding the KE, and the remaining terms describing some forms of PE. This \( E \) is equivalent to values yielded by the common E norm expressed for a model on a periodic Cartesian grid (Ehrendorfer and Errico 1995; cf. Talagrand 1981), except for the normalization by the factor \( A \).

Also conserved is

\[
y = c^T S^{-1} T' - \Pi'
\]

at each \( x, y \) location. Given \( h' = 0 \) and an arbitrary \( y \), or given \( y = 0 \) and arbitrary \( h' \), \( T' \) and \( \Pi' \) are uniquely determined. There is an analogous conserved quantity in the vertically continuous form of (2.1)–(2.6), except the only value of \( T' \) involved is that at \( \sigma = 1 \). In contrast, (2.12) is generally a function of \( T' \) at all levels.

A third conserved quantity is

\[
E^* = \frac{1}{2A} \int_X \int_Y (u'^T Du' + v'^T Dv' + h'^T DH^{-1} h') \, dy \, dx.
\]

(2.13)

It is related to \( E \) and \( y \) by

\[
E = E^* + \frac{1}{2A} \int_X \int_Y R_0 T_x (1 + c^T S^{-1} B^{-1} b)^{-1} y^2 \, dy \, dx.
\]

(2.14)

The term proportional to \( y^2 \) in (2.14) may be interpreted as a portion of UPE in the linearized model expressed by (2.1)–(2.6). It is time independent, neither affecting the wind (since \( h' \) is independent of it) nor affected by it. It is therefore \( E^* \) that may be more properly termed the KE plus APE of (2.1)–(2.6) (although we have not shown that even all that APE can be realized as KE and is therefore actually entirely 'available').

The factor \((1 + c^T S^{-1} B^{-1} b)^{-1}\) in (2.14) is proportional to \((\Delta\sigma)^2\) (or a higher power of \(\Delta\sigma\)) as \(\Delta\sigma \to 0\); i.e. as the vertical resolution increases. This assertion is based on considering that elements of \(c, S,\) and \(B\) are each proportional to \(\Delta\sigma\) but that the number of terms added in the inner product of the two vectors \(c^T S^{-1}\) and \(B^{-1} b\) is equal to the number of model levels, which is inversely proportional to \(\Delta\sigma\). On the other hand, as \(K\) increases, the magnitudes of elements of the vectors \(c^T S^{-1}\) that correspond to the same \(\sigma\)-level tend to constants. These elements also change sign at each adjacent \(\sigma\)-level, which will result in much cancellation of contributions to \(y\) by vertically successive values of \(T'\) if that field is vertically smooth. So, as \(K\) increases, the contribution to \(E\) by the \(y^2\) term will tend to 0. These assertions were confirmed using the two very different vertical finite-difference schemes described by Hack et al. (1993) and Kiehl et al. (1996) for \(10 \leq K \leq 100\).

Since \(E^*\) and \(y\) are conserved independently, any linear combination of the two is also conserved. An infinite number of quadratic invariants of (2.1)–(2.6) therefore exist. Also, analysis of the normal modes of (2.1)–(2.6) (Errico 1989) indicates that each distinct mode conserves its contribution to \(E^*\) independently. Arbitrary quadratic invariants can therefore be formulated by weighting the contributions by distinct modes differently. If all the weights are not identical, the invariant is different than \(E^*\). The speculation by Ehrendorfer and Errico (1995) that \(E\) is the only quadratic invariant of (2.1)–(2.6) is therefore incorrect.

It should be noted that while \(E, E^*\) and \(y\) are invariants of the vertically-discretized primitive equations linearized about an isothermal, resting, flat reference state, they are not necessarily so when linearized about more realistic states. In fact, when using the
E norm to determine leading SVs, the expectation is that \( E \) will increase with time, essentially extracting energy from an unstable reference state (Farrell and Ioannou 1996a,b).

3. Rotational-mode contribution to \( E \)

Since (2.1), (2.2) and (2.9) form a closed system and are linearized about a stationary reference state, they admit normal-mode solutions. One set of solutions are stationary and geostrophic. Their energy contribution, along with that by the complimentary set of gravitational modes, is described by Errico (1989); only an abbreviated description of the geostrophic contribution will be presented here. The presentation employs a spectral representation of the modes, but a corresponding grid-space representation is given by Temperton (1988).

The stationary-mode solutions of (2.1), (2.2) and (2.6) may be described as

\[
(u', v', h') = r_{m,n,\ell} \frac{\sqrt{gH_\ell}}{\lambda_{m,n,\ell}} (in, -im, -f) z_\ell \exp(i mx + i ny),
\]

where \( r \) is a modal amplitude described later, \( g \) is the acceleration of gravity, \( H_\ell \) is an equivalent depth and \( z_\ell \) a corresponding vertical mode (i.e. vertical structure function; also described later), \( m \) and \( n \) are respective wave numbers in the \( x \) and \( y \) directions, \( i = \sqrt{-1} \), and

\[
\lambda_{m,n,\ell} = f \left( 1 + \frac{gH_\ell}{f^2} (m^2 + n^2) \right)^{\frac{1}{2}}
\]

is the frequency of an inertial-gravity wave at the indicated scales. For a periodic domain, \( m \) and \( n \) are products of some integer and \( 2\pi/L_d \), where \( L_d \) is the fundamental periodic wavelength in the respective direction. These modes correspond to the rotational or Rossby mode subset of Hough functions on the sphere (Daley 1991) except, due to the \( f \)-plane assumption, they are rendered stationary. Since (3.1) at all scales is stationary, any linear combination of these modes is also stationary, and their basis for describing the geostrophic components is therefore not unique. The form (3.1), however, facilitates what follows. In particular, this form for the modes provides an orthonormal basis with respect to the \( E \) norm.

The \( z_\ell \) are eigenvectors of \( H \) with \( gH_\ell \) the corresponding eigenvalues (\( \ell = 1, \ldots, K \)). By (2.7) and (2.8), \( D^{1/2}HD^{-1/2} \) is a symmetric matrix, and therefore the \( z \) can be normalized such that

\[
\delta_{k,\ell} = z_k^T D z_\ell.
\]

where \( \delta_{k,\ell} \) is the Kronecker delta. This orthogonality condition can be used to determine vertical-mode coefficients from fields defined on \( \sigma \)-levels. This condition also implies that the wind and \( h' \) fields for each vertical mode contribute independently to the energy expressed by the \( E \) norm.

The \( r \) are determined as

\[
r_{m,n,\ell} = \frac{\sqrt{gH_\ell}}{\lambda_{m,n,\ell}} \left( -inu_{m,n,\ell} + imv_{m,n,\ell} - \frac{f}{gH_\ell} h_{m,n,\ell} \right).
\]

The expression \((-inu + imv)_{m,n,\ell}\) may be interpreted as the component of relative vorticity \( (\zeta') \) orthogonal to the \( \sigma \)-surfaces at the indicated scale, and (3.4) may be
interpreted as an energy-weighted measure of linearized potential vorticity at the given scale.

The complimentary set of modes are those describing inertial-gravity waves. They correspond to the gravitational set of Hough functions and are associated with non-zero values of wind divergence on \( \sigma \)-surfaces and with non-zero ageostrophic vorticity \( \xi' - \nabla^2 h' \), where \( \nabla^2 \) is the two-dimensional Laplacian defined on the \( \sigma \)-surfaces.

The rotational and gravitational modes are mutually orthogonal with respect to the \( E^* \) (or \( E \)) norm such that

\[
E^* = \frac{1}{2A} \sum_{m,n,\ell} r_{m,n,\ell}^* r_{m,n,\ell} + \cdots, \tag{3.5}
\]

where \( r^* \) is the complex conjugate of \( r \) and the missing terms (\ldots) are the contributions by gravitational modes. In this simple model, the orthogonality of the modes implies that the rotational modes are geostrophic and the gravitational modes have zero linearized potential vorticity. The contributions to \( E^* \) by the rotational and gravitational modes will be denoted by \( R \) and \( G \), respectively.

The \( R \) component of \( E^* \) is the value of the \( R \) norm: it is that component of \( E^* \) (or \( E \)) that is contributed to by the rotational (or geostrophic) modes of (2.1)–(2.6). It may be computed by the sequence of operations:

1. Compute \( \xi' \) on \( \sigma \)-levels from \( u' \) and \( v' \), and \( h' \) from \( T' \) and \( \Pi' \), at all \( x, y \) grid-point locations;
2. Project \( \xi' \) and \( h' \) from values defined on \( \sigma \)-surfaces to coefficients of vertical modes at all \( x, y \) grid-point locations;
3. Determine two-dimensional Fourier coefficients (defined in the \( x, y \) directions) of the results of step 2; and
4. Compute \( r \) at each scale using (3.4) (but expressed in terms of \( \xi' \)) and then sum as in (3.5).

The geostrophic component of the fields may be re-constructed from the values of \( r \) by using (3.3) and inverses of the horizontal Fourier and vertical-mode transforms. In order to partition \( h' \) between \( T' \) and \( \Pi' \), the condition \( \gamma' = 0 \) is used.

4. THE \( E \) NORM AND \( R \) NORM INTERPRETED AS COVARIANCES

In the context of ensemble forecasting or predictability studies, perturbations should be constructed that reflect reasonably likely initial-condition errors (Errico and Baumhefner 1987; Anderson 1996). When SVs are used in these contexts, it is therefore appropriate to use an initial norm whose weights are given by the inverse of the covariance matrix describing the uncertainty in the initial analysis (Ehrendorfer and Tribbia 1997; Barkmeijer et al. 1998). For error probability distributions that are a function of such a norm (e.g. under Gaussian assumptions), all SVs may then be considered equally likely. If a norm is defined in terms of a symmetric matrix whose inverse is not expressed explicitly in terms of covariance statistics, but subsequently the norm is considered consistent with such an expression, then the elements of the matrix inverse may be interpreted implicitly as equivalent to those covariance statistics. The \( E \) and \( R \) norms will be interpreted using their equivalent covariance matrices in this section.

Consider a norm applied to the vector of initial conditions \( q \) (e.g. a vector containing all the grid-point values of all the prognostic fields):

\[
J = q^T C^{-1} q, \tag{4.1}
\]
where the elements of \( C \) are the analysis-error covariances between pairs of components of \( q \). The \( E \) norm may be written

\[
E = q^T E q. \tag{4.2}
\]

where \( E \) is the diagonal matrix whose elements are the coefficients before respective fields in (2.11). Equating (4.1) and (4.2) for all \( q \) yields \( C = E^{-1} \), indicating that using the \( E \) norm is equivalent to using a covariance for which there is no correlation between analysis errors at different locations or for different fields. The assumed spectra of the analysis errors for distinct fields within \( q \) are white. Also, the variances for the wind components, \( T \), and \( \Pi \) are 1, \( c_p/T_t \) and \( R_d T_t \), respectively (or, approximately 1 m/s², 0.3 K², and 0.1 kPa², respectively, using \( \Pi' \approx p'/p_{st} \)). Since there is no covariance between any of the distinct fields, there is no assumed difference between variances of vorticity and divergence, no scale preferences, and no dominance of the error variances of rotational components compared with gravitational ones. (This would not be the case if the \( E \) norm were described in terms of other fields; e.g., when described in terms of divergence and vorticity rather than \( u \) and \( v \), the variances of the former are indeed rendered distinct.)

For the covariance that corresponds to the \( R \) norm, there is no strict inverse since the gravitational components of the flow (and \( \gamma \)) are ignored. The pseudo-inverse in the subspace of the rotational modes does exist, however, and therefore it is possible to relate the \( R \) norm to a norm expressed as in (4.1) but restricted to the subspace of geostrophic linearized potential vorticity. In this case it is simplest to relate \( R = \langle r^* r \rangle \) to a corresponding \( \langle q q^* \rangle \), where \( r \) is the vector whose components are \( r_{m,n,\ell} \) and the angle brackets indicate an expectation (e.g., a mean of random values). Here, attention is restricted to \( R \) being diagonal, as it is effectively defined in the \( R \) norm.

In terms of the \( R \) norm, the implied covariance between two elements \( q_a \) and \( q_b \) of \( q \) is

\[
\langle q_a q_b \rangle = \sum_\ell \sum_{m,n} z_{a,\ell} z_{b,\ell} e^{im(x_a-x_b) + in(y_a-y_b)} \alpha_a \alpha_b \langle |r_{m,n,\ell}|^2 \rangle, \tag{4.3}
\]

where indices \( a \) and \( b \) refer to particular grid locations and field types \( u \), \( v \), or \( h \) and

\[
\alpha = \frac{\sqrt{g H_0}}{\lambda_{m,n,\ell}} (-in, im, f) \tag{4.4}
\]

for the respective types of fields. The coefficients appearing in (4.4) are the factors appearing in (3.4). The notation \( z_{a,\ell} \) refers to the component of vertical mode \( \ell \) on the \( \sigma \)-level designated by \( a \).

As an example, consider that \( \langle |r_{m,n,\ell}|^2 \rangle = r_c^2 \) for \( m \leq M, n \leq N, \ell \leq L \), with \( r_c \) a constant. This is the kind of covariance assumed by Ehrendorfer and Errico (1995): a white-noise covariance in a truncated set of rotational modes. In this case,

\[
\langle h_a h_b \rangle = r_c^2 \sum_{\ell=0}^L \frac{g H_0 z_{a,\ell} z_{b,\ell}}{M} \sum_{m=-M}^M \sum_{n=-N}^N \left( 1 + \frac{g H_0}{f^2} (m^2 + n^2) \right)^{-1} \cos(m \Delta x) \cos(n \Delta y), \tag{4.5}
\]
where $\Delta x = x_a - x_b$ and $\Delta y = y_a - y_b$. The other correlations are geostrophically related to this one; e.g.

$$
\langle u_a h_b \rangle = r_c^2 \sum_{\ell=0}^L z_{a,\ell} z_{b,\ell} \sum_{m=-M}^M \sum_{n=-N}^N \frac{ngH_{\ell}}{f} \left( 1 + \frac{gH_{\ell}}{f^2} (m^2 + n^2) \right)^{-1} \cos(m\Delta x) \sin(n\Delta y).
$$

(4.6)

Equations (4.5) and (4.6) are derived by noting that

$$
\sum_{m=-M}^M e^{im\Delta x} = \sum_{m=-M}^M \cos(m\Delta x),
$$

(4.7a)

$$
\sum_{n=-N}^N -in e^{in\Delta y} = \sum_{n=-N}^N n \sin(n\Delta y),
$$

(4.7b)

e tc. In contrast to the E norm, the error covariances implied by the R norm are geostrophic and there are implied spatial correlations. These correlations may be enhanced by truncating the R norm more; i.e. by reducing any of $M, N, L$ and thereby excluding more horizontal or vertical scales from consideration. They may also be enhanced by considering $\langle |r_{m,n,\ell}|^2 \rangle$ that varies with spatial scale indices.

Examples of covariance structures implied by the R norm appear in Fig. 1. They are produced using $H = 100$ m with $L_d = 6000$ km in both horizontal directions, $f = 4\pi \cos(40^\circ)/1$ day and $g = 9.8$ m s$^{-2}$. This value of $H$ was chosen because it describes the typical equivalent depth associated with initial-time leading SVs (Errico 2000). The ranges of $m$ and $n$ appearing in the corresponding sums in (4.5) and (4.6) are truncated such that only

$$
(m^2 + n^2)^{\frac{1}{2}} \leq \frac{2\pi}{L_d} 15
$$

(4.8)

is considered, corresponding to a “circular” truncation at wave number 15 within the domain. Only the horizontal structures appear; the expression $\sum_{\ell} z_{a,\ell} z_{b,\ell}$ in (4.5) and (4.6) has been ignored. The point $b$ is taken as the centre of the domain, and point $a$ is that where the particular covariance is indicated. The value of $r_c^2$ is taken as 1, since we are concerned with only the structure here: $r_c$ may be tuned to give whatever covariance magnitude is desired.

The $\langle h'_a h'_b \rangle$ (horizontal) covariance is shown in Fig. 1(a). Its contours consist of circles centred on point $b$. The corresponding covariance for $\langle u'_a h'_b \rangle$ appears in Fig. 1(b). Note the geostrophy implies that a positive height perturbation at point $b$ is correlated with eastward and westward $u$ perturbations to the north and south of that point, respectively. The magnitudes of the covariances vary greatly between $H = 100$ m and $H = 10^4$ m, as the dominance of the wind or height fields in the rotational modes is altered. The horizontal scales of the various covariances also vary somewhat with equivalent depth (not shown).

The covariances implied by the R norm look similar to the corresponding covariances assumed for short-term, extratropical forecast errors used in current data-assimilation schemes for numerical weather prediction (e.g. Phillips 1986; Daley 1991). Indeed, it may be possible to tune the assumed $\langle |r_{m,n,\ell}|^2 \rangle$ as a function of $m$, $n$, $\ell$,
and even to include consideration of some gravitational-mode covariances so as to construct a norm corresponding more to those specified for data assimilation. Better, however, would be to define a norm with corresponding covariance that looks more like an assumed analysis error. Presumably, this would have smaller scale and be more ageostrophic than those assumed for forecast errors, since the gravest portions of the latter should be partially corrected by observations. It would also be a challenge to mimic the effects of spatially inhomogeneous observations in such a contrived norm (see Barkmeijer et al. (1998) for another approach).

5. MODEL AND CASE

SVs will be computed using the discrete forms of both $E$ and $E^*$ as well as $R$ applied to version 2 of the Mesoscale Adjoint Modeling System (denoted as MAMS2) developed at the National Center for Atmospheric Research (NCAR, Errico and Raeder 1999). It uses the primitive equations within a regional domain with relaxation lateral boundary conditions (Davies and Turner 1977). Its discretization satisfies (2.8). Diabatic processes include vertical and horizontal diffusion, bulk formulation of the planetary boundary layer, dry convective adjustment, and a prognostic surface temperature over land. Moist diabatic processes include convective and stratiform precipitation and radiative effects of clouds on the land surface temperature. A nonlinear normal-mode initialization is applied to the two deepest vertical modes following Bourke and McGregor (1983). Its tangent linear and adjoint versions required for SV determination are exact except for some minor approximations applied for computational efficiency as described by Errico and Raeder (1999). See Errico et al. (1994) for a full description of its parent model: MAMS1.

The tangent linear and exactly corresponding adjoint models are determined using a reference state that is both time and space varying. That state is determined from a forecast produced with the moist version of the model, including full physics. The case covers the 24-hour period beginning 0000 UTC 14 February 1982. The dry dynamics is
dominated by a cyclone that greatly intensifies as it propagates north-eastward along the Atlantic coast of North America. Further details about this case, including the effects of moist diabatic processes on both the forecast and its linearization, appear in Ehrendorfer et al. (1999) and Errico and Raeder (1999).

The SVs have been determined using $T_i = 270\ \text{K}$ and $p_t = 100\ \text{kPa}$, $R_d = 287\ \text{J K}^{-1}\ \text{kg}^{-1}$, and $R_d/c_p = 0.287$. The model grid spacing is 120 km (on a Lambert conformal grid) with prognostic fields defined on ten, equally-spaced $\sigma$-levels. Since the MAMS2 formulation is in terms of $p_s$ rather than $\Pi$, $p'_s/p_{sr}$ replaces $\Pi'$ in the formulations of $E$ and $h$. The SVs determined for the $E$ norm are identical to those discussed by Ehrendorfer et al. (1999).

The MAMS model top is the 1 hPa surface, rather than 0 as assumed throughout section 2. The vertical modes, and hence the rotational, gravitational, and $\gamma$ components, are determined using the actual model top, rendering them inconsistent with the specification of the $E$ norm in section 2. Experiments were performed with a model top closer to 0, to ascertain that this discrepancy is insignificant for the analysis and comparisons performed here. Also, the partitioned modes are computed consistently with the MAMS2 model formulation, thereby retaining an appropriate orthogonality condition. In particular, the MAMS2 formulation satisfies the orthogonality condition for vertical modes.

Another problem faced when comparing the $E$ and $R$ norms in practice is that the MAMS2 wind and thermodynamic fields are defined on two (i.e. staggered) grids with distinct sizes. This yields different fundamental wavelengths for the two grids, and incompatible Fourier modes for the two types of fields. While there are many ways to constrain the problem further, none are natural in the MAMS2 framework. Here, the approach is simply to compute the rotational modes from the vorticity rather than wind fields. This vorticity is defined on the same grid as the thermodynamic variables and determined by finite differences within the staggered grid framework. For the transformation from $r$ to wind, first the stream function is calculated spectrally, and then the wind by finite difference. Furthermore, only a half-range Fourier sine transform is used, since the perturbation fields are constrained to vanish, rather than be periodic, on the lateral boundaries. The expression $m^2 + n^2$ appearing in (3.2) and (4.8) is formulated accounting for these finite-difference approximations as

$$\frac{1 - \cos(m \Delta x) \cos(n \Delta x)}{2(\Delta x)^2}$$

which is the spectral-space coefficient corresponding to application of the MAMS2 5-point Laplacian to a sine wave of scale $m$, $n$ for a conformal map having $\Delta x = \Delta y$ but ignoring the map scale factor. This formulation has a very slight effect except on the smallest scales, but makes the results more consistent with the finite differences used. Note that horizontal variations of the grid map scale factor are ignored in both the $E$ and $R$ norms since it varies throughout the domain by only a few per cent. These choices have also been partly motivated by a desire to use existing MAMS2 software in the $R$-norm computations unless obviously inappropriate.

The SVs determined here are solutions to the problem: maximize $q_1^T N q_1$ given $q_1 = M q_0$ and the constraint $q_0^T N q_0 = 1$, where $q$ is the model state vector describing initial (subscript 0) and final (subscript 1) perturbations, $M$ is the matrix describing the linearized model, and $N$ is the positive-definite symmetric matrix operator defining the norm. The solution is most easily determined as $q_0 = N^{-1/2} p$, with $p$ the leading eigenvector of the symmetric matrix $N^{-1/2} M^T N M N^{-1/2}$. The leading eigenvector is
the one associated with the greatest eigenvalue. Successive SVs may be determined that are orthogonal (with respect to the norm denoted by N) to all the previously determined eigenvectors. Since, for realistic models, the large matrix M exists only as an operator in the form of a computer code, the p are best obtained using an iterative Lanczos algorithm (Strang 1986; Grimes et al. 1994) that does not require an explicit representation of the model operator.

6. DRY RESULTS

SVs with respect to four norms are considered here: the E, E*, and two versions of the R norm. One version of the R norm includes all vertical modes and resolved horizontal scales; the other, denoted as the truncated R norm, excludes small vertical and horizontal scales similar to the formulation by Ehrendorfer and Errico (1995). Although the linearization has been performed about a solution of the nonlinear model that included moist physics, here only linearization of the dry physical and dynamical terms are considered by the tangent linear model and its adjoint.

The leading six SVs have been determined with respect to each norm using enough iterations of a Lanczos algorithm (Strang 1986; Grimes et al. 1994) to achieve their converged solutions. The corresponding singular values appear in Table 1. The E values are identical to those appearing in Ehrendorfer et al. (1999) for their case W2.

(a) E vs. E* norms

The E and E* norms are compared as a step in understanding the R norm. Singular values for the E* norm are typically only a few per cent smaller than corresponding ones for the E norm as shown in Table 1. Structures of corresponding perturbation wind fields of the initial-time SVs are almost identical. At $\sigma$-levels where the initial $T'$ fields have large magnitude, structures for corresponding SVs are also very similar. The only notable differences occur at $\sigma$-levels where the $T'$ fields have very small magnitudes (e.g. near the model top). There the E*-norm SVs tend to have larger magnitude (but still small with respect to levels where it is a maximum) with a noticeable component that changes sign each successive $\sigma$-level.

This alternation of sign is consistent with the effect of filtering the $\gamma$ mode from the E-norm SV. If the temperature is to be altered to make $\gamma$ vanish while preserving $h'$, according to (2.6), the change to $T'$ must have the vertical structure given by $B^{-1}b$, which in the MAMS2 formulation has signs that alternate at successive $\sigma$-levels. In
fact, if the $\gamma$ mode is filtered from the E-norm SV, the result is almost identical to the $E^*$-norm SV at all levels for all fields.

The effects of ignoring the $\gamma$ mode in the SV calculations are not very significant. Significant differences between the E-norm and R-norm results may therefore be interpreted as primarily due to the filtering of gravitational modes and the neglect of any rotational modes that may be omitted (i.e. truncated) from the norm.

(b) $E$ vs. $R$ norms

The leading singular value determined for the R norm is 83% that for the E norm, meaning the ratio of growths of the respective norms is only 0.69. If growth of the leading SV determined for the R norm is measured instead using the E norm, so that the energy of all components are summed at the end time, the growth is still only 75% that for the E-norm SV. Apparently, adding some gravitational (or $\gamma$) components to the R-norm SV structure initially can act to increase growth beyond that indicated by the R norm. This result will be further explored in another paper that explicitly examines the dynamical balance of SVs. Here, it suffices to state that the growth obtained using the R norm is less than that obtained using the E norm, but growths for both are large.

Samples of the structures of the leading E-norm and R-norm SVs at $t = 0$ appear in Fig. 2. The corresponding $u'$ components at all levels look very similar (correlations above 0.9), although the amplitudes may be scaled differently. The same is true for the $u'$ components (not shown), although slightly less so. In the upper levels, where the E-norm $T'$ fields are small, the corresponding R-norm fields closely resemble those of the $E^*$ norm (correlations above 0.9) as opposed to those of the E norm. At the level ($\sigma = 0.55$) where $T'$ is largest, the R-norm and E-norm $T'$ fields are very similar. The corresponding $p'_k$ fields have some commonality, but they are not as similar as other corresponding pairs are. The structure of the initial-time, R-norm leading SV is therefore very similar to that of the corresponding E-norm SV. The same can be said for the pair of second SVs (not shown).

The fractions of $E$ contributed separately by KE (labelled as K) and by the $T'$ contribution to APE (labelled as T) for each $\sigma$-level appear in Fig. 3. Note that the sum of all graphed values is less than 1 because the contribution to $E$ by $\Pi'$ is not shown. The fractions include factors of $(\Delta \sigma)_k = 0.1$ (independent of $k$). At the initial time (Fig. 3(a)), although the $T$ contributions peak at the same level, that peak is less pronounced for the R-norm SV. For KE, magnitudes for the R-norm structure are larger at all levels, by as much as a factor of 2 in mid-atmosphere, so that the R-norm SV is not as strongly dominated by $T$ perturbations at $t = 0$ compared with the E-norm SV. Note that the E-norm result is similar to some aspects of results shown by Buizza et al. (1997); in particular, $E$ peaks just below mid-atmosphere and the contribution by KE is less than that due to APE.

The similarity between the subspaces of the first ten initial-time SVs for the E and non-truncated R norms is indicated in Table 2. It shows projections of R-norm structures onto E-norm structures measured using the E norm. Note that each R-norm SV projects dominantly onto one E-norm SV (projection greater than 0.5). For the first eight SVs, the dominant projection is onto the SV having the same index. The similarity index (as defined by Buizza (1994)) for these two subspaces is 0.68.

At $t = 24$ h, structures of pairs of corresponding leading SV fields generated using the E and R norms are correlated at approximately 0.99. The amplitudes of the R-norm structures, however, are smaller than those for the E norm, commensurate with the ratio of their singular values. The E-norm structure at $t = 24$ h is presented by
Figure 2. The (a) and (b) \( v' \) on \( \sigma = 0.45 \) and (c) and (d) \( T' \) fields on \( \sigma = 0.55 \) at \( t = 0 \) for (a) and (c) the leading singular vector (SV) determined for the R norm and (b) and (d) the E norm. Both SVs are determined for the dry version of the linearized model. Contour intervals are 1 m s\(^{-1}\) and 1 K, for \( v' \) and \( T' \), respectively. Zero-contours are omitted and dashed lines show negative values. See text for further explanation.

Figure 3. Fractions of \( E \) contributed by wind (curves labelled K) and temperature (curves labelled T) fields on each \( \sigma \)-surface for R-norm (dashed line) and E-norm (solid line) singular sectors (SVs) at (a) \( t = 0 \) and (b) \( t = 24 \) h. The values of \( E \) used for normalization are the corresponding ones determined for each distinct SV and time. See text for further explanation.
both Ehrendorfer et al. (1999) and Errico and Raeder (1999). The vertical distribution of KE and APE at \( t = 24 \) h appear in Fig. 3(b), with each of the SV structures normalized so that \( E = 1 \). Results are nearly identical for the two norms, and are similar to those reported for typical final-time SVs described by Buizza et al. (1997); in particular, \( E \) peaks in the upper half of the atmosphere and is primarily in the form of KE.

(c) \( R \) vs. truncated \( R \) norms

The truncation considers only the smaller half of values of either \( m \) or \( n \), so that only approximately 1/4 of the combinations of wave numbers are included. This corresponds to ignoring wavelengths shorter than \( 4\Delta x \) in either direction. Also, the shallowest three vertical modes, corresponding to \( H_L < 10 \) m, are neglected. These scales are ignored because it was originally assumed that they are strongly affected by diffusive damping and therefore can contribute little to growth, and because without such significant truncation the implied vertical and horizontal correlation scales shrink to those of the grid spacing.

The singular values in Table 1 reveal that the leading SV determined for the truncated R norm grows less than for the non-truncated R norm. As for the R vs. E-mode SVs, this is due to the two reasons that (1) a portion of the perturbation is not measured at the final time when using the truncated norm and (2) some potentially growing structure is excluded at the initial time. For these two leading SVs, it is again the latter that explains most of the results. In particular, it is the excluding of vertical mode 8 that accounts for most of the discrepancy.

The truncated R-norm structures for the leading SV at \( t = 0 \) appear in Fig. 4 for comparison with the structures appearing in Fig. 2. Corresponding structures are similar in shape except for a noticeable broadening of the SV in the truncated case.

Projections for the initial truncated R-norm SVs onto the E-norm SVs appear in Table 3. As for the R-norm SVs, the projection is dominantly onto the same-indexed SV. The magnitude of the dominant projection is smaller, however, indicating that the spatial truncation has altered the structures more. The similarity index for this subspace is 0.41.

7. MOIST RESULTS

Only the E and non-truncated R norms are considered in this section. Since these norms do not measure moisture explicitly, the initial moisture perturbation fields are
appropriately constrained to be zero (Ehrendorfer and Errico 1995). The full-physics versions of the tangent linear and adjoint models are used. The E-norm results are identical to experiment W4 of Ehrendorfer et al. (1999). The leading five singular values for the two sets appear in Table 1. There is little similarity between values having the same indices. The three leading SVs for the E norm are shown by Ehrendorfer et al. (1999) to be associated with convection over Mexico. The next two SVs are associated with the developing cyclone in the Atlantic. The structures of these last two modes correspond well with those for the leading two SVs with respect to the R norm.

As an example, the $\nu'$ and $T'$ fields on $\sigma = 0.55$ at $t = 0$ for the leading moist SV produced with the R norm and the fourth SV produced with the E norm are presented in Fig. 5. They appear well correlated, which is a characterization describing $\nu'$ on all $\sigma$-levels, and $T'$ on all levels where it is relatively large (as for the $E^*$ and E-norm comparisons with the dry linearization). The growth of the R-norm SV is only 57% of the E-norm SV when measured using the respective norms.

Errico and Raeder (1999) and Errico (2000), show that the leading E-norm SV in this moist model is dominated by gravitational modes. The R norm therefore effectively filters this mode from its leading SVs. The same appears true for other convectively-driven growth that is associated with primarily ageostrophic dynamics. The R norm can therefore serve as a filter of ageostrophic convective SVs if that is deemed desirable.
Figure 5. The (a) and (b) $v'$ on $\sigma = 0.45$ and (c) and (d) $T'$ on $\sigma = 0.55$ at $t = 0$ for (a) and (c) the leading singular vector (SV) determined for the R norm and (b) and (d) the fourth SV for the E norm. Both SVs are determined for the version of the linearized model that includes moist diabatic physics. Contour intervals are (a) 2 m s$^{-1}$, (b) 1 m s$^{-1}$, (c) 1 K, and (d) 2 K. Zero-contours are omitted and dashed lines show negative values. See text for further explanation.

8. Conclusions

In the context of the simple linearized model from which it is derived, the E norm has the significant property that it is a quadratic invariant, although it is not the only such invariant. This invariance is lost when it is applied to more realistic reference states or models (i.e. those including diabatic physics). If that were not so, it would be useless for determining 'growing' components of the flow because, for that purpose, a norm that can change with time is required. Although it is called a measure of energy, it has not been demonstrated that it is indeed such in the contexts to which it has been applied. The fact that it has units of energy per unit mass does not by itself qualify it as a measure of energy.

Although the E norm is a sum of KE plus a portion of PE in the context of the simple linearized model, it is not the KE plus APE in vertically discretized forms of that model. Some of the PE it measures is unavailable. As the vertical resolution increases, however, this unavailable portion tends to vanish. Also, when the model linearization is instead performed about more realistic states, neither the available nor unavailable portion of PE measured by the norm remains precisely that; i.e. with a more general basic state, portions of both can be transformed to KE.

A norm that measures only the portion of energy contributed by rotational modes is introduced as the R norm. In MAMS2, these modes are components of geostrophic
linearized potential vorticity. If the R norm does not include a spectral truncation, the size of the state vector it measures is slightly less than 1/3 that for the E norm. If the norm also ignores some horizontal scales or vertical modes, the size of this vector is further reduced.

The E norm and R norm can be interpreted in terms of respectively equivalent norms expressed as quadratic measures of perturbation fields with weights given by the inverse of analysis-error covariance matrices. In the case of the E norm, this covariance matrix is diagonal; i.e. there are no cross correlations in space or between fields. In contrast, the covariance matrix equivalent to the R norm has implied spatial correlations. Furthermore, between different field types it has implied geostrophic correlations. Such correlations are similar to error correlations assumed for short-term forecast errors, although it is unclear how they may be related to covariances of analysis errors. The R norm can be tuned to change these implied correlations either by, vertically or horizontally, spectrally truncating its definition or by assuming different spectra of rotational-mode weights. It is also easy to extend it to include some consideration of gravitational-mode components of the fields.

Without applying additional scale-dependent weights to the R-norm definition, the R norm measures the energy at all scales equally within the subspace to which it applies. In this sense it is like the E norm but different from the inverse Hessian norm or inverse background-error covariance norm of Barkmeijer et al. (1998). Those latter norms effectively weight the initial total energy at larger scales less than at smaller ones, thereby favouring initial perturbations at larger scales.

The leading R-norm SVs are co-located with corresponding E-norm SVs when both are produced using the dry linearized model. At their initial time, corresponding horizontal structures in terms of individual fields and model levels have similar shapes, but their relative magnitudes are very different. In particular, the magnitudes are such that the E-norm SV is obviously not exactly geostrophic initially (whereas all R-norm SVs are). One notable exception to the similarity of structure is the temperature field near the model top, where the corresponding structures are uncorrelated and have greatly different amplitudes. For SVs for either norm, however, the temperatures at these levels are clearly sub-dominant.

At hour 24, for which the SV growths were optimized, shapes of the SV structures produced by the two norms are almost identical (correlations at 0.99). The amplitude of the hour 24, R-norm SV is smaller than that of the E norm, although both SVs have grown much when measured using either norm. The growth of the R-norm SV is less than that of the E-norm SV because the former SV lacks some ageostrophic component that accelerates growth in the latter.

When moist physics is considered by the linearized model, the R norm effectively filters the leading ageostrophic, convectively forced SVs obtained using the E norm. Structures of the corresponding remaining leading SVs are similar, as with the dry-model results. The growth is less for the R-norm SVs than for the E-norm SVs, although growths of both are significantly enhanced by the moist physics.

The R norm is a useful alternative to the E norm for some applications. It can be used to imply correlated analysis-error covariance statistics. It can be used to filter some convectively-dominated instabilities from results when linearized moist physics is considered. Especially when used in a spatially truncated form, its SVs can be described in a much reduced model space, which can facilitate determination of a larger portion of the spectrum of R-norm SVs. The additional effects of gravitational modes on the E-norm SV results is described by Errico (2000) and it is hoped that the determination of a larger proportion of the R-norm SVs will be described in a subsequent paper.
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APPENDIX

Example expressions of $\mathbf{B}$ and $\mathbf{c}$

Different models may have very different expressions for their vertical finite-difference operators. Shown here is one set of such expressions, as used by MAMS2 (Errico et al. 1994; Errico and Raeder 1999) as derived from Community Climate Model version 2 (Hack et al. 1993). When its top boundary is defined to be at $p = 0$, the $k$th elements of the MAMS2 $\mathbf{u}$, $\mathbf{v}$, $\mathbf{T}$, $\mathbf{D}$, and $\mathbf{h}$ fields are the two-dimensional portions of the respective fields specified on the surface of constant $\sigma = \sigma_k$, with $k = 1, \ldots, K$ indicating an ordering from the top-most data level to the one nearest the surface.

In MAMS2, with $p = 0$ as the upper boundary, the elements $B_{k, \ell}$ of the matrix $\mathbf{B}$ are defined as

$$B_{k, \ell} = \begin{cases} 
0, & \ell < k, \\
\frac{R_d}{2} \ln \left( \frac{\sigma_{k+1}}{\sigma_k} \right), & \ell = k, k < K, \\
\frac{R_d}{2} \ln \left( \frac{\sigma_{\ell+1}}{\sigma_{\ell-1}} \right), & \ell > k, k < K, \\
\frac{R_d}{2} \ln \left( \frac{1}{\sigma_{K-1} \sigma_K} \right), & \ell = K, k < K, \\
\frac{R_d}{2} \ln \left( \frac{1}{\sigma_K} \right), & \ell = K, k = K.
\end{cases}$$

(A.1)

The operator $\mathbf{c}$ is defined by the vector with elements

$$c_k = - (\Delta \sigma)_k,$$

(A.2)

where $(\Delta \sigma)_k = \sigma_{k+\frac{1}{2}} - \sigma_{k-\frac{1}{2}}$, with half-values indicating the interfaces between atmospheric layers ($\sigma_{k+\frac{1}{2}} > \sigma_{k+\frac{1}{2}} > \sigma_k$, $\sigma_{\frac{1}{2}} = 0$, and $\sigma_{K+\frac{1}{2}} = 1$). From $\mathbf{B}$ and $\mathbf{c}$, $\mathbf{S}$ and $\mathbf{b}$ are determined by (2.8) and (2.7), respectively.

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