

A comparison of Lyapunov and optimal vectors in a low-resolution GCM

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ABSTRACT

We compare the first local Lyapunov vector (LLV) and the leading optimal vectors in a T10/18 level truncated version of the National Centers for Environmental Prediction global spectral model. The leading LLV is a vector toward which all other perturbations turn and hence it is characterized by the fastest possible growth over infinitely long time periods, while the optimal vectors are perturbations that maximize growth for a finite time period, with respect to a chosen norm. Linear tangent model breeding experiments without convection at T10 resolution show that arbitrary random perturbations converge within a transition period of 3 to 4 days to a single LLV. We computed optimal vectors with the Lanczos algorithm, using the total energy norm. For optimization periods shorter than the transition period (about 3 days), the *horizontal* structure of the leading initial optimal vectors differs substantially from that of the leading LLV, which provides maximum sustainable growth. There are also profound differences between the two types of vectors in their vertical structure. While the 24-hour optimal vectors rapidly become similar to the LLV in their vertical structure, changes in their horizontal structure are very slow. As a consequence, their amplification factor drops and stays well below that of the LLV for an extended period after the optimization period ends. This may have an adverse effect when optimal vectors with short optimization periods are used as initial perturbations for medium-range ensemble forecasts. The optimal vectors computed for 3 days or longer are different. In these vectors, the fastest growing initial perturbation has a horizontal structure similar to that of the leading LLV, and its major difference from the LLV, in the vertical structure, tends to disappear by the end of the optimization period. Initially, the optimal vectors are highly unbalanced and the rapid changes in their vertical structure are associated with geostrophic adjustment. The kinetic energy of the initial optimal vectors peaks in the lower troposphere, whereas in the LLV the maximum is around the jet level. During the integration the phase of the streamfunction field of the optimal vectors, with respect to their corresponding temperature field, is rapidly shifted 180°. And, due to drastic changes that also take place in the vertical temperature distribution, the maximum baroclinic shear shifts from the lower troposphere to just below the jet level. Just after initial time, when the geostrophic adjustment dominates, the leading optimal vectors exhibit a growth rate significantly higher than that of the LLV. By the end of the period of optimization, however, the growth rate associated with the leading optimal vectors drops to or below the level of the Lyapunov exponent. The transient super-Lyapunov growth associated with the leading optimal vectors is due to a one-time-only rapid rotation of the optimal vectors toward the leading LLVs. The nature of this rapid rotation depends on the length of the optimization period and the norm chosen. We speculate that the initial optimal vectors computed with commonly used norms may not be realizable

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perturbations in a dynamical system (that is not forced by random noise) since the leading optimal vectors are directions in the phase space from which perturbations are "repelled". By contrast, the leading LLV is the vector toward which all random perturbations, including the optimal vectors, are attracted, which gives the LLV a unique role in linear perturbation development.

1. Introduction

The study of atmospheric instabilities predates the theory of dynamical systems. For example barotropic instability associated with horizontal shear in a basic zonal flow was studied by Kuo (1949) and Lorenz (1972), baroclinic instabilities related to vertical shear in the basic current by Charney (1947) and Eady (1949), and instability of currents with horizontal and vertical shear by Pedlosky (1964) and Brown (1969). More recently, the interest in the nature of instabilities that can lead to fast perturbation growth arose again, partly motivated by the need to better understand the processes that lead to fast and dramatic developments in the atmosphere (Farrell, 1988). Also, it has become clear that in present operational forecast systems the atmospheric analyses used as initial conditions may contain errors associated with fast growing modes (Toth and Kalnay, 1993, denoted TK93 hereafter) and Rabier et al. (1994). If the fast growing modes can be identified, they can be used as initial perturbations in ensemble forecasting, representing those possible error patterns that can cause the largest deviation from the control forecast (Molteni and Palmer, 1993, TK93). Moreover, once identified, the fast growing modes can also be at least partially removed from the analysis via 4-dimensional variational data assimilation (Rabier et al., 1993), or through a simple adjustment of the first guess along the growing modes (Kalnay and Toth, 1994, denoted as KT94 hereafter).

In the analysis of fast growing modes, a method originally proposed by Lorenz (1965) in meteorology has been recently applied in a number of studies. Lorenz' method allows computation of the fastest growing perturbations on either a constant (Farrell, 1988) or a time dependent flow (Lacarra and Talagrand, 1988), for a *prespecified time interval*, and with respect to a *prechosen norm*. In recent applications, these perturbations, denoted "optimal vectors" or "singular vectors" have been determined by the Lanczos algorithm,

which is an iterative application of the forward and adjoint versions of linear tangent models (Lacarra and Talagrand, 1988; Houtekamer, 1991, 1995; Barkmeijer, 1992; Buizza et al., 1993).

While these growing perturbations, optimized for short periods of time, are of interest on their own, in dynamical systems theory attention has been focused more on error growth associated with the Lyapunov vectors. The leading Lyapunov vectors are directions in the phase space that provide the fastest growth on the attractor that can be sustained for long periods of time (Legras and Vautard, 1996). Their growth is sustainable because it is measured after all transient effects died out, and is measured by the Lyapunov exponents. Unlike optimal vectors, the leading Lyapunov vector is independent of the choice of norms or time intervals, indicating that it is more general in nature. The amplification factors associated with optimal vectors and Lyapunov vectors were recently compared by Trevisan and Legnani (1995) for a three variable Lorenz system. They found that the very high, "super-Lyapunov" growth rate of the optimal vectors takes place only for a short period of time at the beginning of the optimization period, after which the amplification rate quickly drops to the value of the Lyapunov exponent.

There have been many theoretically oriented studies of the Lyapunov exponents of simple systems, but the Lyapunov vectors of very large systems, such as those of a high resolution general circulation model of the atmosphere, were estimated for the first time by TK93. They proposed a simple and inexpensive approach, "breeding of growing vectors" (BGV), which is based on multiple runs with a fully nonlinear model, to estimate the Lyapunov vectors of the atmosphere. The basic idea behind the BGV method is that, after a transient period of time, all quasi-linear perturbations turn into the subspace of the leading local Lyapunov vectors (LLVs, see eq. (16) and associated discussion for a formal definition). With this method it is feasible to compare the optimal

vectors that give the largest amplification for a short time period to the Lyapunov vectors that represent the fastest sustainable growth.

Singular vectors and estimates of the leading Lyapunov vectors (bred vectors) are used in the operational practice of numerical weather prediction at major forecast centers. The initial perturbations that are applied on the control analysis for initiating an ensemble of forecasts to represent the uncertainty in a prediction are determined by the singular vector approach and the breeding method at ECMWF and NCEP, respectively (see, for example, Molteni et al., 1996, and TK93). Therefore, a comparison between the Lyapunov and optimal vectors, which is the main topic of this paper, may give an insight into the differences and similarities of the two different approaches. For the comparison we use a highly truncated version of the National Centers for Environmental Prediction (NCEP, formerly National Meteorological Center) Medium-Range Forecast (MRF) model. In section 2, we discuss the definition of the optimal and Lyapunov vectors and the basic methodology to compute them. Section 3 describes the numerical experiments and the results of the comparison between the two types of vectors. In section 4 we present some conclusions and a discussion, including possible implications for the practical application of growing vectors in the analysis of the atmosphere and in generating initial perturbations for ensemble forecasting.

2. Definitions and methodology

2.1. Tangent linear evolution of perturbations

The stability properties of dynamical systems are traditionally characterized by the evolution of infinitesimally small perturbations developing on the nonlinear trajectory of the system. The well known definitions below are given in the context of a tangent model linearized upon the nonlinear model trajectory.

For the duration of a medium-range forecast, the atmospheric equations discretized in space form an N -dimensional system of ordinary differential equations:

$$\frac{dx}{dt}(t) = F(x(t)), \quad x = (x_1, \dots, x_N), \quad F = (F_1, \dots, F_N), \quad (1)$$

where x denotes the real vector of discretized prognostic variables and F is a nonlinear real vector valued function of the same vector variable. If the original model variables are complex they could be easily transformed to a real state vector x . The local dynamics via the evolution of small perturbations $z(t)$ (represented by a column vector) along any reference orbit $x(t)$ can be described by the tangent-linear system of equations

$$\frac{dz}{dt}(t) = J(t)z(t), \quad (2)$$

where the Jacobian matrix J represents the $\partial F / \partial x$ derivative tensor (Tabor, 1989).

The solution of (2) is a linear mapping from the space of initial perturbations $z(t_0)$ to the space of perturbations at time t , $z(t)$:

$$z(t) = R(t, t_0)z(t_0), \quad (3)$$

where R is the resolvent matrix. On the basis of the theory of singular value decomposition (SVD, Golub and Van Loan, 1983, p. 70–72) one can prove the existence of

$$U = [u_1, \dots, u_n] \in R^{n \times n}, \quad V = [v_1, \dots, v_n] \in R^{n \times n} \quad (4)$$

orthogonal matrices such that

$$U^T R V = \Sigma, \quad \Sigma = \text{diag}(\sigma_1, \dots, \sigma_n) \in R^{n \times n} \quad (5)$$

where

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n \geq 0. \quad (6)$$

The orthogonality of U and V means that

$$U^T U = I \in R^{n \times n}, \quad V^T V = I \in R^{n \times n}. \quad (7)$$

It follows that $[u_1, \dots, u_n]$ and $[v_1, \dots, v_n]$ form orthonormal bases for R^n if the inner product and the norm is defined by the euclidean inner product

$$\langle a, b \rangle = a^T b = \sum_{i=1}^n a_i b_i, \quad \|a\|^2 = \langle a, a \rangle.$$

The $\sigma_i (i=1, \dots, n)$ are the singular values of R and the vectors u_i and v_i are the i th left and right singular vectors respectively. From the SVD theory we know that

$$R v_i = \sigma_i u_i. \quad (8)$$

Since $[v_1, \dots, v_n]$ is an orthonormal basis for R^n , an arbitrary $z_0 = z(t_0)$ can be written as

$$z_0 = \sum_{i=1}^n \langle v_i, z_0 \rangle v_i. \quad (9)$$

Making use of eqs. (3), (8) and (9),

$$z(t) = R z_0 = \sum_{i=1}^n \langle v_i, z_0 \rangle R v_i = \sum_{i=1}^n \langle v_i, z_0 \rangle \sigma_i u_i. \quad (10)$$

Multiplying (10) by u_i

$$z(t) u_i = \langle v_i, z_0 \rangle \sigma_i, \quad (11)$$

one can see that

$$\sum_{i=1}^n \frac{\langle z(t), u_i \rangle^2}{\sigma_i^2} = \sum_{i=1}^n \langle v_i, z_0 \rangle^2 = \|z_0\|^2 = 1. \quad (12)$$

It follows that the singular values of the matrix R are equal to the length of the semi-axes of the hyperellipsoid E defined by

$$E = \{R z_0 : \|z_0\| = 1\}, \quad (13)$$

and the orientation of the semi-axes in the phase-space is defined by the left singular vectors of R .

2.2. Lyapunov characteristics

2.2.1. Global Lyapunov exponents. The Lyapunov characteristics of a dynamical system describe the long-term evolution of the hyperellipsoid E . As time goes to infinity, the mean growth of the principal axes of this hyperellipsoid defines the global Lyapunov exponents (Tsonis, 1992):

$$\lambda_i = \lim(s \rightarrow \infty) \frac{1}{s} \ln(\sigma_i(t_0 + s)). \quad (14)$$

As can be seen, there are as many Lyapunov-exponents as the dimension of the phase-space. Out of the spectrum, the largest global Lyapunov exponent is the most important one and is representative of the stability of the system along a long trajectory. In particular, if a system has at least one positive Lyapunov exponent, its behavior will be chaotic; arbitrarily close trajectories will diverge with time till they become completely independent. In contrast, the behavior of a system with negative Lyapunov exponents can be predicted for infinitely long time periods.

It has been shown theoretically that the Lyapunov exponents exist for Hamiltonian systems (Benettin et al., 1976). On the basis of Oseledec's multiplicative ergodic theorem, Benettin et al. (1976) also proved that for these systems the quantity:

$$\lambda_1 = \lim(s \rightarrow \infty) \frac{1}{s} \ln \left(\frac{\|z(t_0 + s)\|}{\|z(t_0)\|} \right) \quad (15)$$

is equal to the largest Lyapunov exponent for almost all $z(t_0) = z_0$. Shimada and Nagashima (1979) carried out numerical experiments with the 3-variable Lorenz model (Lorenz, 1963) to investigate the above problem for dissipative systems. Their results show that the Lyapunov exponents also exist for the 3-variable Lorenz model. For large forced-dissipative systems the existence of Lyapunov exponents can only be demonstrated by numerical experiments.

The first global Lyapunov exponent can be computed by integrating the tangent-linear system of (2) for a long period of time with random initial conditions. During the integration the quantity of (15) converges to the first Lyapunov exponent. Note that to avoid computational overflow, renormalization of the linear perturbation vector may be necessary during the extended integrations (Benettin et al., 1976).

2.2.2. Local Lyapunov exponents and vectors.

Though the global Lyapunov exponents describe a system's long term stability properties, they provide no information on how instability changes locally in the phase space. However, this information may be crucial for practical applications, since in general, the orientation and the stretching/contracting properties of the perturbation hyperellipsoid change continuously as the hyperellipsoid moves along the trajectory of the system. To describe these changes in instability on the attractor, the Lyapunov exponents can also be defined locally (Nese, 1989; Trevisan and Legnani, 1995):

$$I_1(x) = \lim(\tau \rightarrow 0) \frac{1}{\tau} \ln \left(\frac{\|z(t+\tau)\|}{\|z(t)\|} \right) \quad (16)$$

$$= \frac{d}{dt} \ln(\|z(t)\|), \quad t > T,$$

after the transient behavior of the initial perturbations died off. Beyond the first local Lyapunov exponent one can also define the whole spectrum of exponents. At any point on a trajectory the exponents are associated with the basis of the time dependent orthogonal vectors u_i , $i = 1, \dots, n$ (the orientation of the perturbation hyperellipsoid after infinite time evolution), which are the *local Lyapunov vectors* (LLVs) of the system. Note that the local Lyapunov exponents and vectors are defined at a particular point on the attractor (hence their name "local"), but they contain

information from the trajectory of the system preceeding that point. Ideally, the perturbations should be introduced infinite time earlier before the local Lyapunov characteristics are evaluated. In practice, strong convergence is found when the perturbations are introduced some finite time before they reach a particular point on the attractor. The length of this time period depends on the dynamics of the system in question.

By definition, the first LLV, which is independent of the norm definition, represents the direction in which maximum sustainable growth (or least decay) can occur in a system without external forcing. In fact, after a finite transition period T all random* initial perturbations turn into the direction of the leading LLV at any given point on a trajectory. Consequently if we are interested in estimating not only the first but also the successive local Lyapunov exponents we need to periodically reorthogonalize u_i 's (Shimada and Nagashima, 1979; Benettin et al, 1980; Wolf et al., 1985; Vannitsem and Nicolis, 1994). In practice the local Lyapunov exponent(s) are estimated with respect to a predefined finite time period τ as

$$L(x(t), \tau) = \frac{1}{\tau} \ln A(t, \tau), \quad A(t, \tau) = \frac{\|z(t+\tau)\|}{\|z(t)\|}, \quad (17)$$

where the ratio $A(t, \tau)$ is the *local amplification factor*.

2.2.3. Nonlinear extension. TK93 have extended the notion of Lyapunov characteristics into the nonlinear domain. In their method, called the breeding of the growing vectors (BGV), they use the full nonlinear version of the NCEP Medium Range Forecast (MRF) model to estimate instability properties of the atmosphere. For this purpose, two integrations are carried forward upon the evolving analysis fields (or a long model integration). The control forecast starts from the analysis, while the perturbed forecast starts from an arbitrarily perturbed analysis. After a short period of time (of the order of a day) the difference between the perturbed and unperturbed control forecasts

is rescaled to the size of the initial perturbation, and this rescaled difference is reintroduced onto the corresponding new analysis field. This procedure, if applied iteratively, is analogous to running a nonlinear perturbation model, in which the perturbation amplitudes are kept in a band of amplitudes.

TK93 first studied the LLV's of such a complex system as the atmosphere. In the breeding method, they used a perturbation amplitude that is characteristic of the magnitude of actual errors in the atmospheric analysis. In this case, the bred vectors, which are a combination of the leading LLVs, offer a tool for modeling error evolution in the analysis cycle (KT94.) Furthermore, TK93 found that the transition period after which initially random perturbations converge to the leading LLVs is 3-4 days for the atmosphere. The power of the breeding method lies in this fact: with only a few days of nonlinear model integration the Lyapunov characteristics of the flow can be successfully estimated.

As an additional step beyond traditional instability analysis where the emphasis is on the computation of *Lyapunov exponents*, the estimates of the leading *local Lyapunov vectors* from breeding have been studied and used in operational practice. To express the uncertainties in weather forecasts due to the combined effect of imperfect analysis and the chaotic nature of the atmosphere, an ensemble of weather forecasts is created at NCEP daily replacing the earlier practice of running only one control forecast (see also Tracton and Kalnay, 1993.) The initial perturbations in the ensemble are created by running multiple breeding cycles (Toth and Kalnay, 1996; hereafter referred to as TK96).

TK93 and TK95 pointed out that the use of the nonlinear breeding method is especially crucial in case of complex systems where there are different physical processes operating on different time scales. In this case, instabilities of different nature arise (e. g., convective instability, in addition to baroclinicity), which are associated with different growth rates and different nonlinear saturation amplitudes. For example, TK93 found that with perturbation amplitudes representative of analysis uncertainty, the bred vectors for the atmosphere primarily consist of baroclinic instabilities: convective modes, though they grow much faster, saturate at energy levels lower than the

* If there is a fixed point in a system with a stable subspace, a zero measure set of perturbations will not converge to the first LLV. An example for the 3-variable Lorenz system can be found in Shimada and Nagashima (1979).

perturbation amplitude and thus do not dominate the bred vectors. So by choosing an appropriate perturbation amplitude, the breeding method can estimate the Lyapunov vectors associated with different scales of motion in a complex system.

The use of a strictly linear approach under these circumstances may lead to serious errors in assessing the overall instability of a system. If all physics of a complex system like the atmosphere are considered, a linear analysis would find small scale convection as the leading instability of the flow. However, for regional and global analysis and forecast errors, these instabilities are not dominant since they can attain only small amplitudes in a realistic, nonlinear environment. For the sake of simplicity, nevertheless, we will follow a linear approach in the current study when comparing the LLVs and the optimal vectors. Furthermore, since our focus is on regional and global numerical weather forecasting, we limit our attention to baroclinic instabilities by using linear tangent and adjoint models without convection.

2.3. Optimal vectors

Whereas LLVs represent the vectors associated with maximum sustainable growth, special directions can be constructed in which growth can exceed that associated with the LLVs for a short finite time period and with respect to a prechosen norm. The optimal perturbation z_{opt} is the initial vector with a fixed length $\|z(t_0)\|$ that provides the largest linear amplification $\|z(t_0 + T_{\text{opt}})\|/\|z(t_0)\|$ for a given period T_{opt} with respect to a predefined norm. According to Subsection 2.1 the norm is defined here by the Euclidean inner product. Using the SVD theory

$$\begin{aligned} \|z(t)\|^2 &= (Rz_0)^T(Rz_0) = z_0^T R^T R z_0 = z_0^T V \Sigma^2 V^T z_0 \\ &= \sum_{i=1}^n \sigma_i^2 \langle v_i, z_0 \rangle^2. \end{aligned} \quad (18)$$

This means that the ratio $\|z(t)\|/\|z(t_0)\|$ is maximal if and only if $z(t_0) = v_1$, or in other words the optimal perturbation z_{opt} is equal to the first right singular vector of R . In this sense the i th right singular vector could be termed as the i th optimal vector. The optimal vectors describe the short-term evolution of the perturbation ellipsoid E , which depends on the initial perturbation. At the end of the optimization period T_{opt} the shape of an optimal vector v_i is defined by u_i , while the

amplification factor is given by σ_i . At this time the vectors $\sigma_i u_i (i=1, \dots, n)$ are orthogonal to each other. For an infinite long optimization period, the mean logarithmic growth rate of the i th optimal vector is equal to the i th Lyapunov exponent and the i th optimal vector turns into the direction of the i th local Lyapunov vector.

Lorenz (1965) proposed a simple algorithm for the computation of optimal perturbations. It can be easily shown that the right singular vectors of R are the eigenvectors of the $R^T R$ matrix, while the singular values are the square roots of the eigenvalues for the same vectors:

$$R^T R v_i = \sigma_i^2 v_i. \quad (19)$$

This equation provides a straightforward algorithm for the computation of the right singular (optimal) vectors. Here R^T , the transpose of R , represents R^* , which is the adjoint of operator R , defined by the Euclidean inner product $\langle a, Rb \rangle = \langle R^*a, b \rangle$. Consequently, the expression $R^T R z_0$ is equivalent to the integration of the tangent linear model and a subsequent integration of the linear adjoint model for the initial perturbation z_0 .

For large problems, the most effective way to compute these eigensolutions is through the use of the Lanczos algorithm (Golub and Van Loan, 1983, and for meteorological applications: Laccara and Talagrand, 1988, Houtekamer, 1991, Buizza et al., 1993, Buizza and Palmer, 1995). In practice, the Lanczos algorithm involves a large number of iterations, in each of which we first integrate the tangent linear, and then the linear adjoint of the model, for a time period that is equal to T_{opt} . For example, in order to obtain 30 singular vectors optimized for 36 h at T21 horizontal resolution, about 100 iterations are needed, equivalent to about 300 days of integration (Molteni et al., 1996.)

The resulting optimal vectors are very sensitive to the choice of the optimization period and norm (Vukicevic, 1993.) Applying a proper scaling operator W to the vector of model variables the Euclidean inner product may define any quadratic quantity as norm. Beyond obvious choices for the norm such as pseudo energy (generally referred to as total energy, Buizza, 1993), one can introduce other specific norms. By doing so, the perturbations can be confined at either the initial or the final time to certain statistical or dynamical characteristics. For example, Ehrendorfer and Errico (1995) used a norm that emphasizes rotational

kinetic energy on the larger scales. Houtekamer and Derome (1995) used a norm that eliminated structures that are alien to the statistical characteristics of estimated analysis errors while Buizza (1994a), through the introduction of a local projection operator, computed optimal vectors that amplify over a predefined geographical region. Derber (personal communication, 1994) has suggested that a norm representing an estimate of the analysis/forecast error covariance matrix is preferable to the more commonly used energy norms for analysis applications. The range of choices regarding the length of the optimization period and the norm, and the sensitivity of the optimal vectors to these choices, suggest that the optimal vectors are very particular properties as opposed to the general nature of the Lyapunov vectors. This statement is accentuated by the fact that all random perturbations (including the optimal vectors themselves) turn into the direction of the leading LLV.

3. Numerical experiments

3.1. Numerical models

All the experiments reported here were carried out using a version of the 18 level NCEP MRF model (Kanamitsu et al., 1991) truncated at a low horizontal resolution of T10 (equivalent to a Gaussian grid size of about 1300 km at the Equator), with a time step of 30 minutes. The tangent linear and adjoint versions of the full nonlinear model were coded for the adiabatic version of the NCEP MRF model, but the effects of the horizontal diffusion and a simple surface drag parametrization were also included (Navon et al., 1992). Without some surface friction parameterization in the linear tangent model, fast growing perturbations were observed in the optimal vectors near the surface layer by Buizza (1994b). These perturbations, however, did not grow within the full nonlinear model with physical parameterizations.

3.2. Basic trajectory

The full nonlinear truncated MRF model was integrated for an extended period (100 days), starting from initial conditions corresponding to the NCEP analysis at an arbitrary date (April 3,

1992), and this integration was used as a basic trajectory for the computation of the LLV and the singular vectors. The stability computations were carried out for different periods within these 100 days, but since the results obtained were similar in all cases, we will discuss only those corresponding to the period centered on day 95 of the integration. The streamfunction field corresponding to day 95 is shown in Fig. 1a. By this time in the course of the nonlinear integration, the flow assumed a pattern that is representative of the model attractor: a strong zonal current with relatively small amplitude traveling waves. The height-latitude cross-section of the zonal wind of the flow is shown in Fig. 1b. It is the Southern Hemisphere, wintertime jet stream that is stronger and as we will see below, this is that supports the dominant instability of the flow.

3.3. Computation of the LLV

As described above the leading LLV (hereafter referred to as LLV) can be estimated by linear breeding with a simple integration with the linear tangent model. The linear model was integrated 15 times from well balanced, independent random initial perturbations, for time periods ending at and after day 95. No renormalization was necessary (see Subsection 2.2.1) since no numerical overflow occurred in our experiments. After a 3-5 days transient period, the initially independent perturbations converged to the same horizontal and vertical structure. After 20 days of linear integration, most of the 15 perturbations were found to be essentially identical (except for the sign, which is arbitrary) by visually inspecting them and also by projecting them onto each other, via different inner products. This convergence is confirmed by the comparison of the amplification factors associated with the 15 independent linear breeding experiments (Fig. 2). All this indicates that the linearly bred growing vectors converge to a well-defined LLV, corresponding to the dominant instability of the flow. These results correspond well with the findings of Houtekamer and Derome (1994, 1995.)

The LLV at day 95 is presented in Fig. 3a. The well organized wavenumber 6 pattern in the Southern Hemisphere prevails throughout most of the vertical domain of the atmosphere, both in the streamfunction and temperature fields. Only

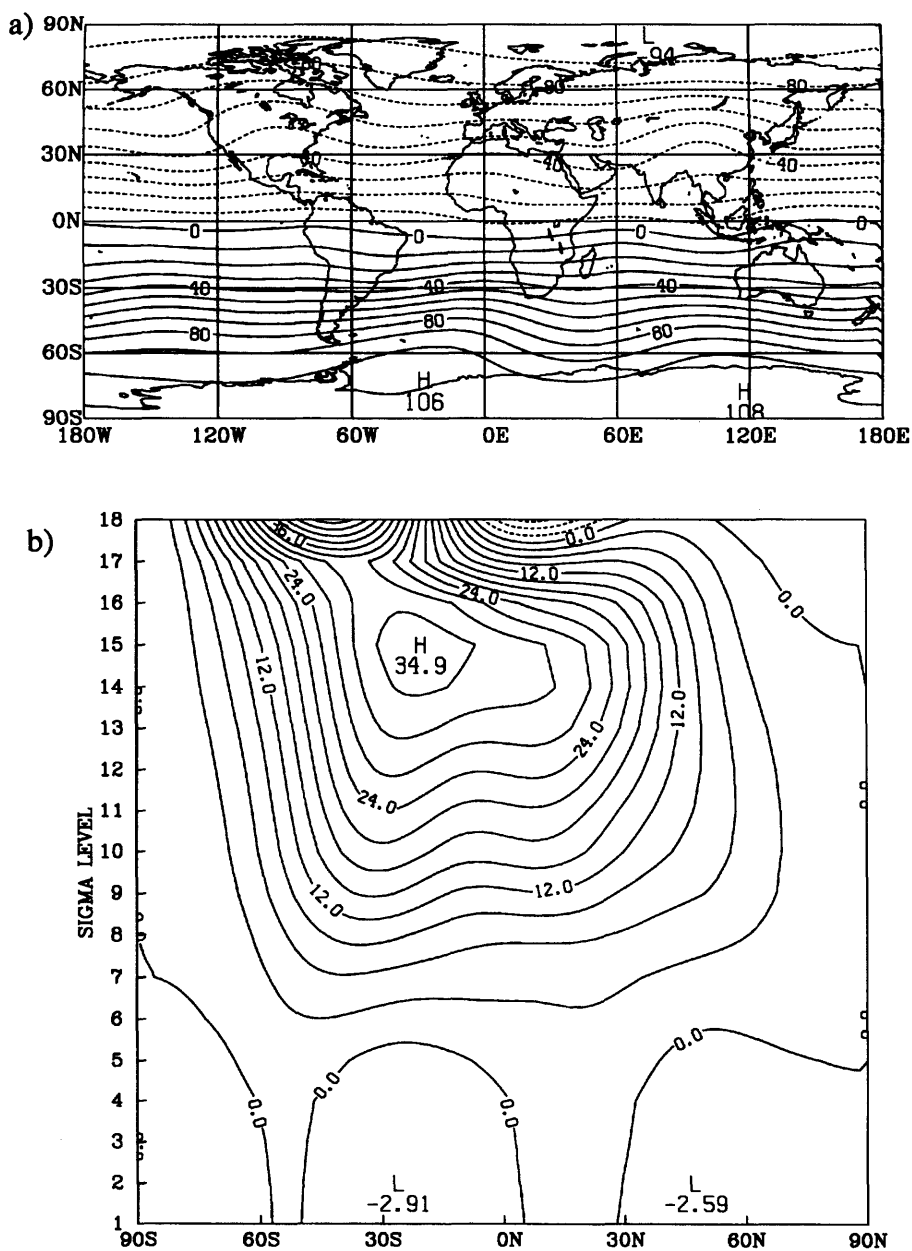


Fig. 1. The 500 hPa streamfunction field after 95 days integration with the nonlinear model. This field defines the background flow at beginning of the different long optimization periods (a). The height-latitude cross-section of the zonal wind in the background flow after 95 days nonlinear model integration (b).

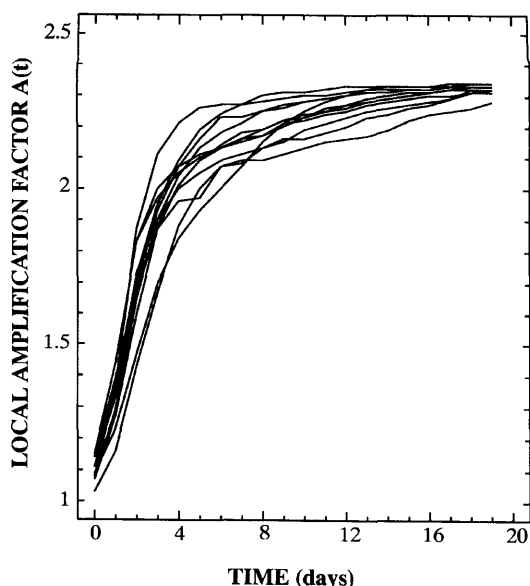


Fig. 2. The time evolution of the local amplification factors for the initially independent random perturbations with an updating frequency of 24 h. The figure shows the amplification factors between the 75th and the 95th day of the nonlinear model integration.

at the topmost layer the streamfunction field contains larger scales. In order to carry out the comparisons described in later parts of this section, the LLV was also computed for each day between days 95 and 100 (Fig. 3b). We note that in simple systems higher order Lyapunov vectors may have a larger local amplification than that of the leading LLV (Trevisan, 1993; Vannitsem, 1995, personal communication). However, when we computed a large portion of the LLV spectrum in a separate study, we have not noticed such a behavior in the T10 MRF.

While in simple linear systems like our T10 model, and in certain conditions (specifically, when there is a dominant instability in the system) a unique leading LLV exists, there is no guarantee that such a unique solution can be experimentally found at any given computational accuracy for more complex systems. We note that experiments with nonlinear perturbation models (breeding) show no clear sign of convergence to a *single* vector either at the present low resolution (T10) or at a higher T62 resolution (TK93, TK96).

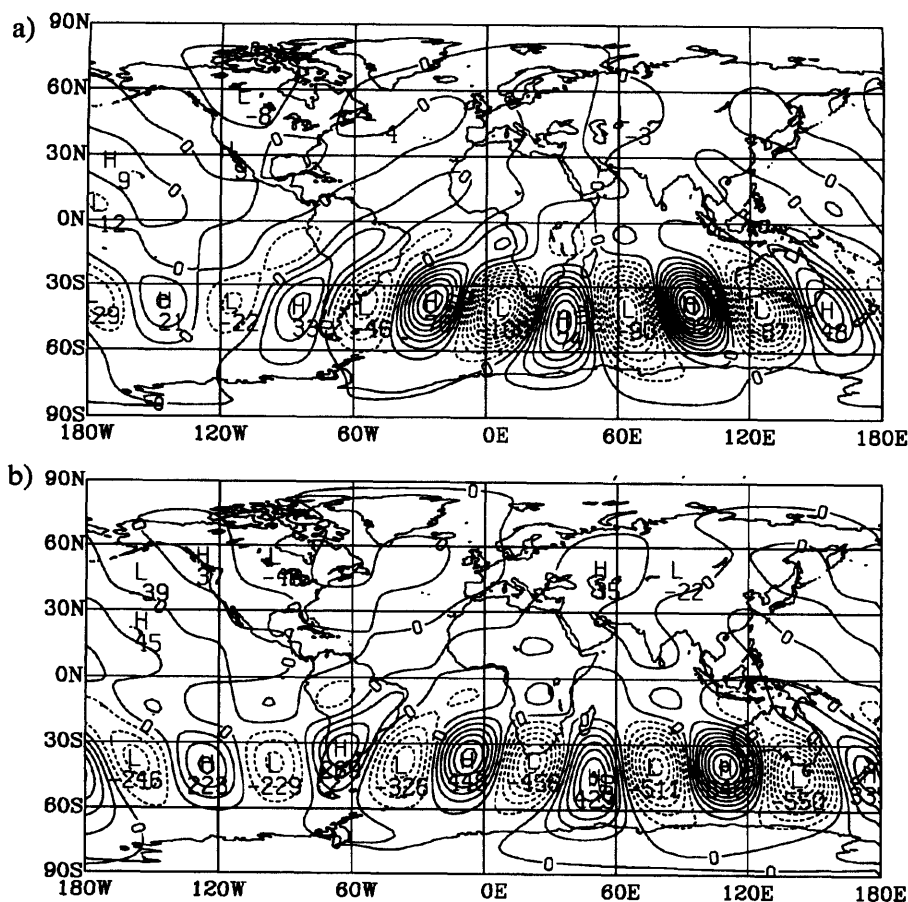
Some experiments were carried out using the

nonlinear BGV algorithm. Due to the very high truncation of the model, even at high perturbation amplitudes the dominant instability was convection associated with tropical modes. These tropical diabatic instabilities did not converge to a single mode but rather to a few dominant patterns. Since in the atmosphere and in more realistic GCMs large scale tropical disturbances have lower growth rates than baroclinic mid-latitude instabilities, the tropical modes observed in the T10 MRF nonlinear perturbation fields are an artifact of the unrealistic climate of this highly truncated version of the model. Therefore we present only the linear results pertaining to baroclinic mid-latitude modes (that are also observed as the leading instabilities in nonlinear breeding experiments with more realistic models).

3.4. Computation of the optimal vectors

As mentioned above, the definition of the singular or optimal vectors is dependent on the norm used. For generating initial ensemble perturbations, the norm should ideally be selected such a way that the analysis error have a white noise distribution, i. e., using that norm, errors in all phase space directions would be equally likely. This could be achieved by using the analysis error covariance matrix — a matrix that is hard to estimate. As a step in this direction, Houtekamer (1995) considered vertical covariance estimates when defining his SVs. Molteni et al. (1996) compared three commonly used norms and found that the total energy norm violates the least the white noise requirement when verified in only one direction (wavenumber spectrum) of the phase space. One should note, however, that commonly used norms such as rms or total energy norm do not satisfy the white noise error distribution requirement since they contain no information from the analysis error distribution.

In this study, partly for the sake of a comparison with the operational practice followed at ECMWF, we follow Buizza et al. (1993) and use the total energy as a norm (and associated inner product.) We use Talagrand's (1981) formulation with the addition of a constraint to ensure that the initial perturbations have unit amplitude with respect to this norm. It should be noted that the total energy defines a norm only if the perturbations have a zero mean. We made sure that all of



(i.e., more widely different amplification factors.) In our experiments the eigenvectors appeared in pairs. The structure (and associated eigenvalue) of the two paired vectors are practically identical but they are out of phase by 90° . Hence, the computation of, for example, 10 eigenvectors, yields only 5 independent (differently shaped) initial perturbations (optimal vectors). In the following the eigenvectors are numbered by pairs, except where noted otherwise.

As an example we show first the singular vectors for a 24-h optimization period. The first singular vector, which is the perturbation growing fastest over the 24-h period, has a structure of wavenumber seven (Fig. 4a). This structure is present at all layers of the model atmosphere except near the upper and lower boundaries. The additional paired vectors have similar features, except that the second vector has a wavenumber 6 structure (Fig. 4b), the third has a less symmetric structure of wavenumber 8 (Fig. 4c), while the fourth has a structure which is a mixture of perturbations with different scales, with wavenumber 8 dominating (Fig. 4d). Another important and general feature of the optimal vectors is that at each level the temperature field (not shown) has a very similar horizontal structure to that of the streamfunction field. The phase difference between the two fields, however, varies from level to level in such a way that the 24-h initial optimal vectors exhibit a *very strong baroclinic shear* (which we will discuss further below and in the Appendix.)

3.5. Comparison between the leading LLV and the optimal vectors

3.5.1. 24-h optimal vectors. To study the time evolution of the 24-h initial optimal vectors, each of them was integrated for 5 days, using the tangent linear model, and starting at day 95, the beginning of the optimization period. Fig. 5 presents the daily amplification factors for the first five vectors. The vectors undergo substantial changes as their amplification factor drops dramatically below that associated with the LLV after the first 24 h of integration. After the initial short-lived super-Lyapunov growth, the horizontal structure of all the optimal perturbations slowly evolves towards the LLV, and their amplification factor approaches (from below) the LLV growth rate. For example, the initial perturbation of vector

3 (wavenumber 8 pattern, Fig. 4c) assumes a pattern reminiscent of the wavenumber 6 pattern of the LLV after 120 h of integration (see Fig. 6). Along with the changes in the perturbation patterns, the relative order of the perturbations, with respect to their associated amplification factor, also changes. For example, vector 2, which initially has the horizontal structure (wavenumber 6) closest to the LLV, grows faster than vector 1 after 48 hours (cf. Figs 3b and 4b).

In addition to the change in the horizontal patterns, there is an equally important change in time in the vertical structure of the optimal vectors. This change is related to the vertical distribution of both their energy and baroclinic shear. This change is associated with a geostrophic adjustment process and takes place at a faster pace than that related to the change in the horizontal shape of the patterns, as we will see later in more detail in connection with the 120-hour optimized vectors (for details, see the Appendix).

3.5.2. 120-h optimal vectors. If we increase the optimization period from 24 to 48 h, the first two optimal vectors are similar to the corresponding 24-h vectors. The third vector has a somewhat irregular wavenumber 7 structure, while the fourth has a structure of wavenumber 5 (not shown.) For 72 h or longer optimization periods the sets of leading optimal vectors are very similar to each other. For the sake of brevity, we will discuss only the 120-h optimization results below. The first four vectors have a wavenumber 6, a slightly irregular wavenumber 7, a wavenumber 5 and a wavenumber 4 structure, respectively (Figs. 7a–d). These structures dominate at all model levels, except at the bottom layer, where the vectors have slightly less organized structure, and at the top layer, where they generally have larger scale structures.

The most important property of the 120-h initial optimal vectors is that the first pair of vectors have a horizontal structure very similar to the LLV but they have a *substantially different vertical structure*. We stress again that this vector is practically identical to the leading optimal vectors determined for any time interval that is 72 h or longer. Apparently, for optimization periods equal to or longer than 72 h, the perturbations, unlike those optimized for shorter periods, cannot extract much extra energy from the flow by assuming an

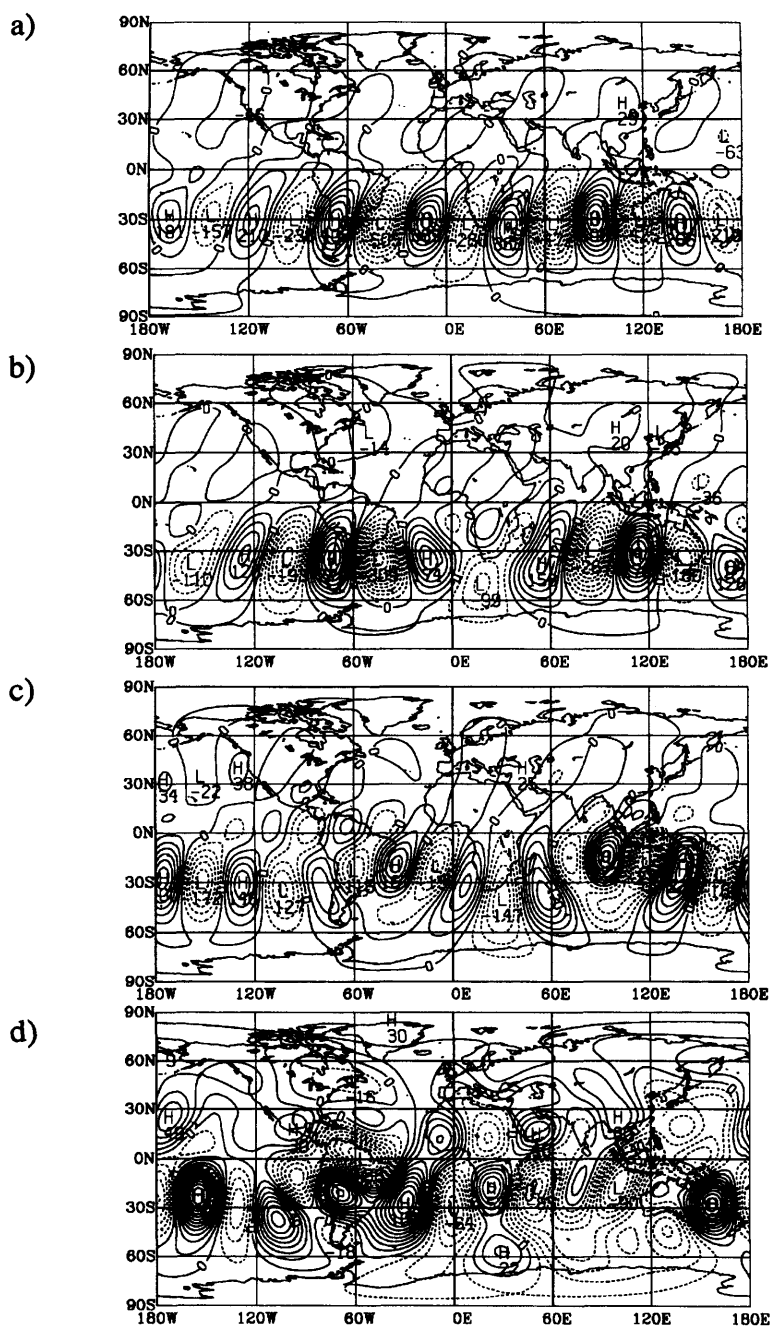


Fig. 4. The first four 24-h optimal modes (500 hPa streamfunction), optimized for a 24-h period started on day 95 of the nonlinear model integration.

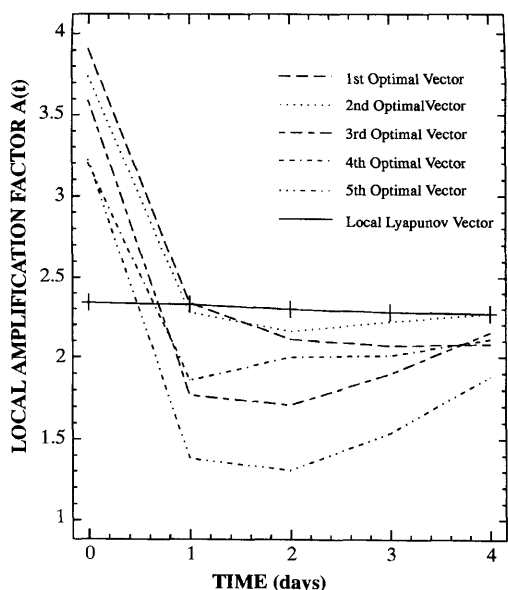


Fig. 5. The time evolution of the amplification factors for the first five 24-hour optimal vectors (500 hPa streamfunction), starting on day 95 of the nonlinear model integration. The solid line indicates the estimated amplification factor for the local Lyapunov vector.

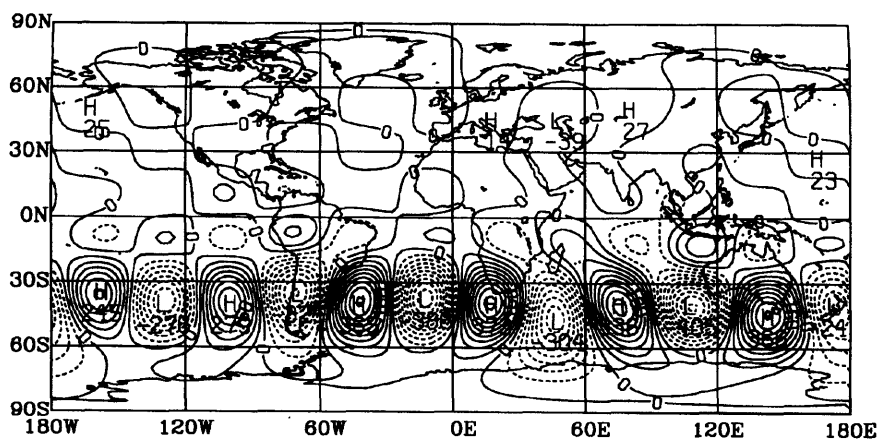
initial perturbation whose *horizontal* structure is different from the LLV. The 72-h limit corresponds well with the time interval it takes for a random perturbation to turn into the direction of the LLV either in this highly truncated T10, or in the T62 version of the MRF (TK93.) The three days time limit is on the order of synoptic time scales

associated with baroclinic instabilities and seems to be an important characteristic of the flow.

Since increasing the length of optimization beyond 72 h makes no appreciable change in the optimal vectors, the first optimal vector for the 120-h optimization can be considered also as an estimate of an *initial* perturbation that is optimal for an *infinite time period*. Note that this perturbation is *different* from the LLV, which is the perturbation that grew optimally in the *preceding* infinite long time period. The difference between the LLV and the first initial optimal vector (that we will discuss below) apparently provides the short-lived super-Lyapunov growth characterizing the leading singular vectors optimized for 72 h or longer time periods.

As mentioned above, the primary difference between the 120-h leading optimal vectors and the LLV is in their vertical structure. While the LLV has a primary kinetic energy maximum at the level of the jet and a secondary maximum near the surface (Fig. 8a), the 120-hour optimal initial perturbations have a maximum in the lower troposphere, at the third sigma level and only a very weak secondary maximum at the jet level (Fig. 8b). A similar structure of the optimal vectors was also documented in a truncated version of the ECMWF primitive equation weather forecast model by Buizza (1994b).

Another important difference between the optimal and Lyapunov vectors is in their vertical distribution of *baroclinic shear*. In the initial optimal vectors, there is very little tilt present in



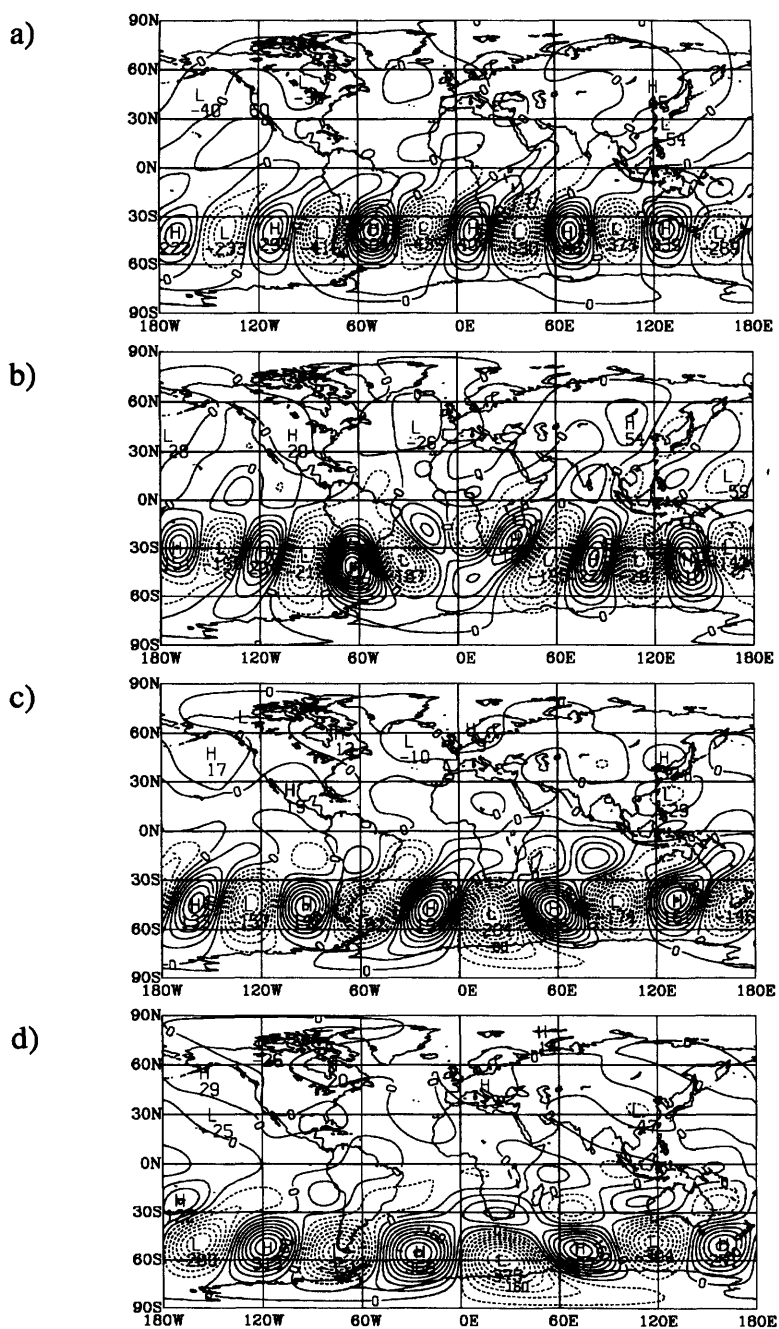


Fig. 7. The first four 120-h optimal vectors for days 95–100 of the nonlinear model integration (500 hPa streamfunction.)

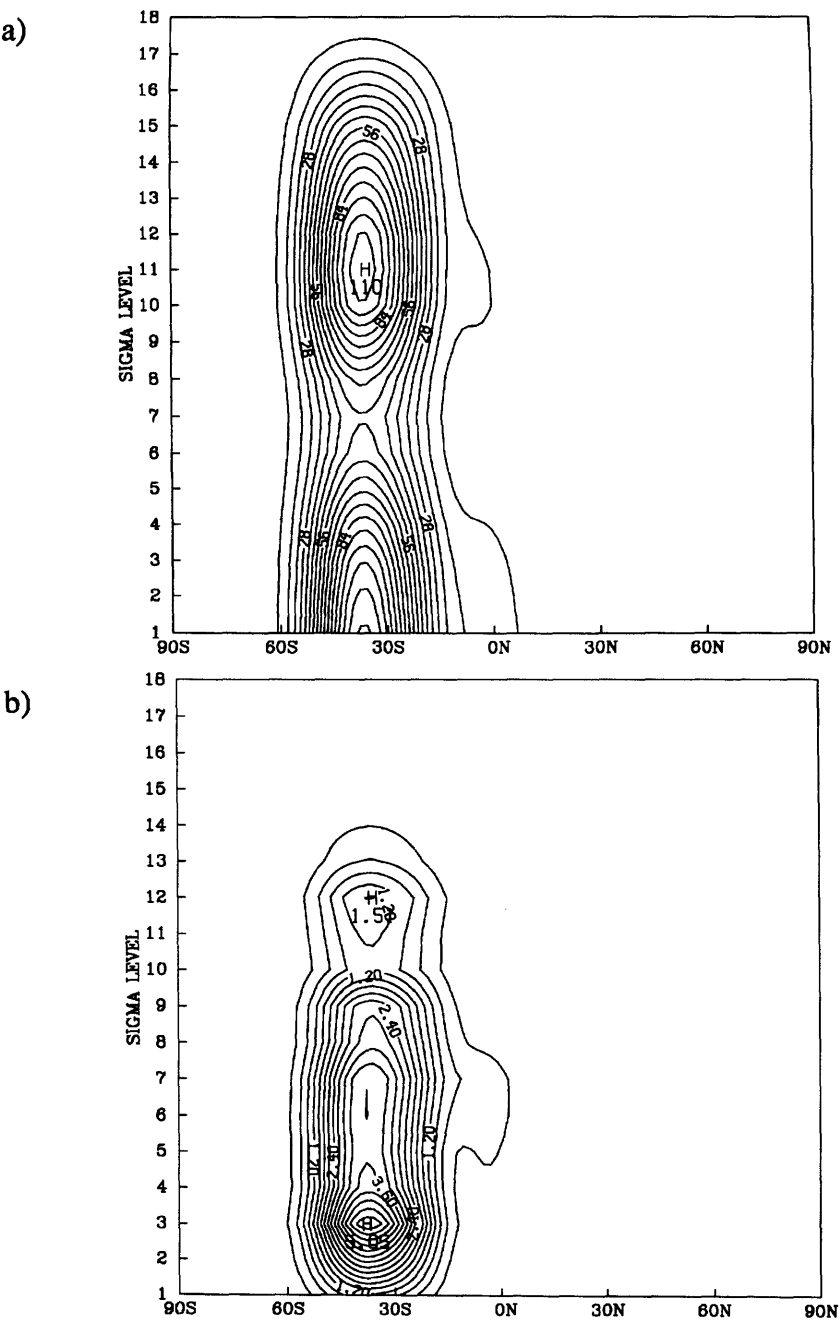


Fig. 8. The height-latitude cross-section of the kinetic energy of the estimated LLV (a) and the 120-h optimal initial perturbation (b) on day 95 of the nonlinear model integration.

the streamfunction field (Fig. 9a) while a strong tilt develops by the end of the 120-hour optimization period (Fig. 9b). It is important to note again that at the end of the optimization period the first optimal vector assumes a structure essentially *identical* to the LLV. In other words, the vertical distribution of the streamfunction field drastically changes in the optimal vectors, resulting in a large growth beyond that exhibited by the LLV. Once this one-time-only change is complete, the maximum attainable growth is that associated with the LLV.

Similar one-time-only changes take place in the vertical distribution of the temperature field. At the initial time, a strong baroclinic tilt is present, centered between levels 7 and 8 (Fig. 10a). At the end of the optimization period, there is no tilt in the lower troposphere. In contrast, the tilt now is at the jet level (between levels 11 and 12), in the region where baroclinic instability has its maximum (Fig. 10b). Comparing Figs. 9a and 10a and then 9b and 10b we can also see that it is the lower troposphere (from the bottom to level 5) where baroclinic shear has its maximum at initial time. In contrast, at the end of the optimization period, the perturbation exhibits its maximum shear around level 10, just below the jet maximum. Note also that the heat advection from the Equatorial region to the poles occurs in a deep layer in the LLV but only in a shallow layer near 780 hPa in the initial optimal vectors (see Fig. 11). The deeper heat transport for the LLV corresponds well with the pattern that is observed in the real atmosphere (see, e.g., Fig. 5.7 in James, 1994) except that our model with its severely limited physics cannot reproduce the drop of heat transport near the surface due to reduced low level wind speed.

This subjective evaluation of the rotation of the initial optimal vectors is well supported by the use of an objective measure, the projection of the optimal vectors on the first LLV, giving the square of the cosine of the angle between the LLV and the optimal vectors (i.e., pattern correlation, PC.) We compare the vertical shear present in the vectors by projecting, with two different norms, the LLV on the subspace of the first few 120-h optimal vectors for all 18 layers. The first projection is obtained using the kinetic energy norm (which is an unbiased inner product in the vector space defined by the vorticity and the divergence

variables, excluding temperature), and the second with the total energy norm (which is an unbiased inner product in the vector space of all model variables, including temperature). A difference between the two projections indicates a discrepancy in the vertical shear between the optimal vectors and the LLV. The kinetic energy norm is also applied to a single layer in which case we measure only the similarity in the horizontal shape of the vectors, irrespective of their vertical structure. The projections were computed at the initial time and then every 24 h up to 5 days. The results, which are presented in Fig. 12, can be easily interpreted since the 120-hour optimal vectors remain orthogonal to each other throughout the optimization period.

We note first that the leading 5-day optimal vector has a horizontal structure very similar to the LLV. The PC with kinetic energy is 0.63 at the initial time and approaches 1.0 at day 5 when measured at a single mid-tropospheric level. Second, considering now also the vertical structure of the vectors, the initial projection of the LLV onto the same first optimal vector is 0.49 with the kinetic energy and only 0.22 with the total energy. The difference between the two PC's indicates that the vertical structure of the temperature field in the first initial optimal vector has a different relationship to the vertical distribution of the streamfunction field from that in the LLV; but this initial difference vanishes within a day. Third, much of the difference between the first optimal vector and the leading LLV disappears by the end of the optimization period (PC=0.93 with total energy). Note that the bulk of the adjustment occurs during the first 24–48 h, during which the optimal vector “releases” much of its extra energy “charged” in its distinctive vertical structure.

If one decomposes the initial optimal vector into a vector parallel and perpendicular to the first LLV, the instantaneous growth in the orthogonal direction is below that of the first LLV. The overall super-Lyapunov growth of the optimal vector, as expected theoretically (Branstator, 1985; Borges and Hartman, 1992), is due to its rotation into a direction where “modal” growth is large, i.e., into the direction of the first LLV. This rotation is well documented in Fig. 12 where the projection of the first 120-h singular vector onto the first LLV changes from an initial value of 0.22 to a final value of 0.93.

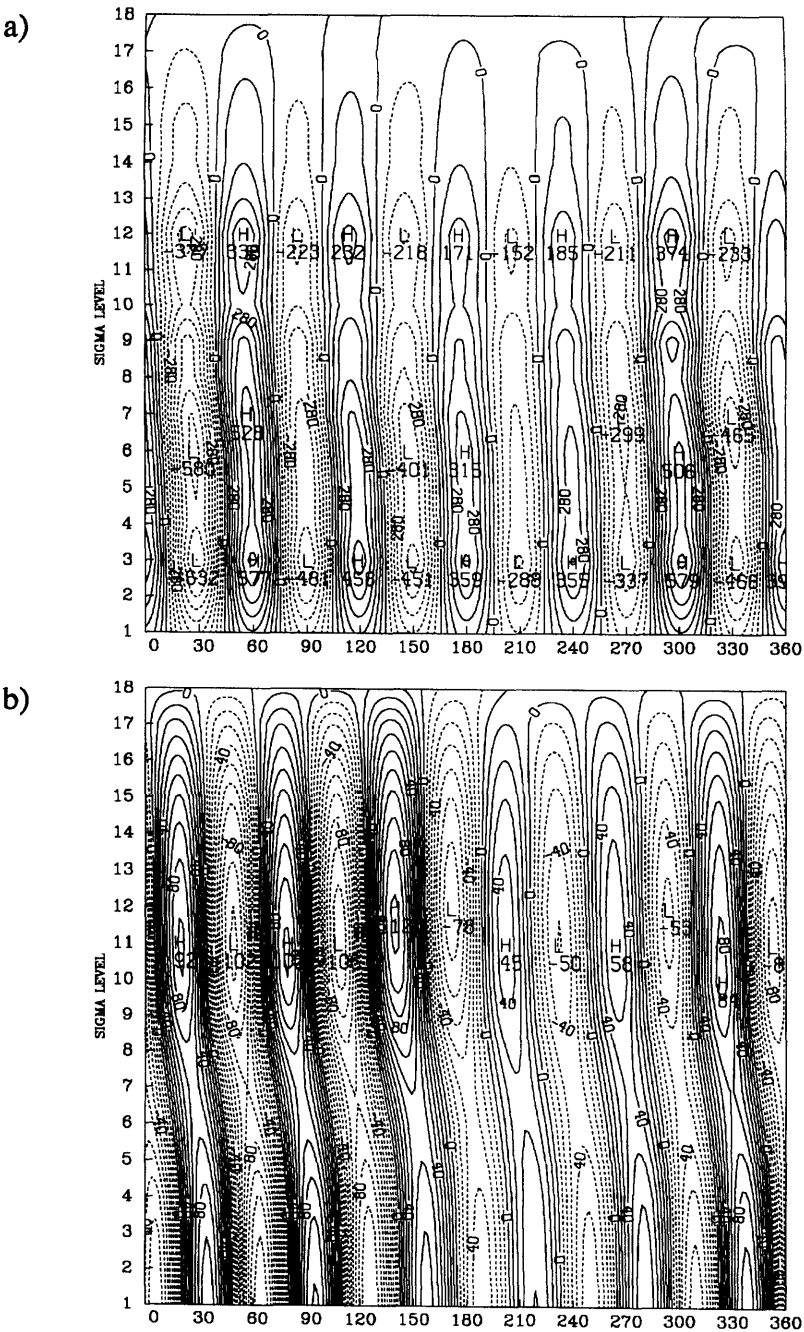


Fig. 9. Height-longitude cross section (at around 50 South latitude) of the streamfunction field for the 120-hour optimized perturbation at (a) initial and (b) final time. Note that (b) is practically identical to the structure of the leading LLV.

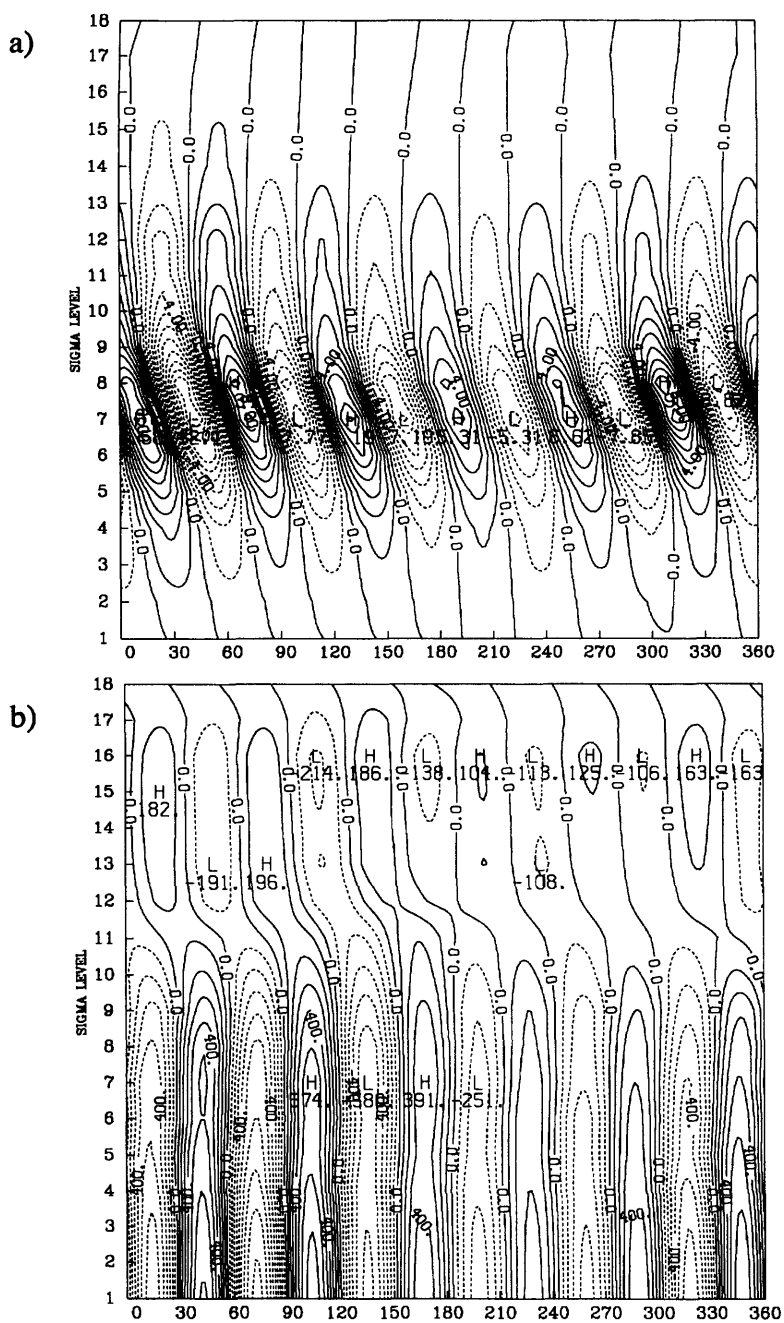


Fig. 10. As in Fig. 9 except for temperature.

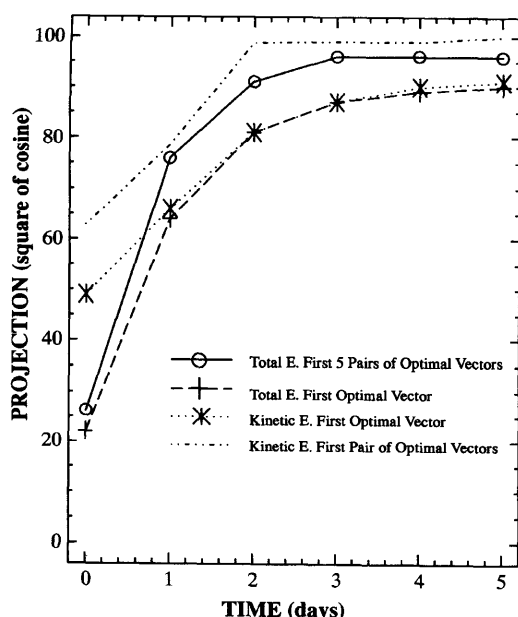


Fig. 12. Time evolution of the projection of the estimated LLV on various subspaces of the optimal vectors with respect to different inner products.

Examination of the thermal wind balance in the optimal vectors and the LLV (see the Appendix for details) reveals that the super-Lyapunov growth of the optimal vectors defined by the total energy norm is primarily due to a geostrophic adjustment process. The initial optimal vectors are actually highly unbalanced in a way that the amplitude of the temperature perturbations in the midtroposphere is about *ten times larger* than that required to keep the balance with the vertical windshear. Consequently, the geostrophic adjustment generates a sudden and large increase in the vertical windshear (kinetic energy). This is the main source of the large initial growth but it is, of course, not sustainable. Note that optimal perturbations even at the initial state transport the heat poleward in the midtroposphere due to the large equatorward meridional temperature gradient in the perturbation at sigma level 7 and 8, hence they can be considered as superbaroclinic instabilities. The vertical structure of optimal vectors converges within a 24 hours period to that of the LLV. In that structure, there is only a slight lack of balance and it is the temperature that

adjusts to the vorticity (streamfunction), and not vice versa, as in the initial optimal vectors.

It is interesting to note that Buizza (1995) compared the rms amplitude of the optimal vectors computed at ECMWF to that of an estimate of analysis errors from the operational OI analysis system. He found that the wind components are *one order of magnitude smaller* in the optimal vectors than in the OI analysis error estimate, while the temperature perturbations have comparable amplitudes. This suggests that the ratio of temperature and streamfunction amplitudes in the ECMWF optimal vectors are, similarly to our findings, unrealistically large, resulting in geostrophically highly unbalanced initial perturbations.

Our results are also in good agreement with those presented by Ehrendorfer and Errico (1995) with a limited area model, using the total energy norm. They also found that the initial evolution of optimal perturbations is associated with the geostrophic adjustment process. They speculated that the total energy norm may give better results for a GCM, with energy conserving vertical differences. Our results, however, do not confirm their speculation. We obtained highly unbalanced initial perturbations, though the vertical differencing of the NCEP MRF is conservative (Sela, 1981).

In summary, for singular vectors optimized for 3 days or longer, the difference from the LLV, responsible for the short-lived initial super-Lyapunov growth, is mainly in the vertical structure of the vectors, due to a geostrophic imbalance in the SVs. This difference is very short lived, though (a day or two) even for 5-day optimized singular vectors. The horizontal shape of the leading optimal vector(s), even at initial time, is similar to that of the LLV. Overall, by the end of the 120-hour optimization period, the first pair of optimal perturbations can explain 93%, while the first 3 pairs can explain close to 100% of the variance in the first LLV.

Finally, in Fig. 13 we present a comparison of the local amplification factor for optimal vectors with different optimization periods, for the first LLV and for fifteen well-balanced random initial perturbations. The local amplification factor for the random perturbations is defined as the average of the amplification factors for the fifteen individual vectors. The one- and two-day optimized singular vectors have large initial growth rates,

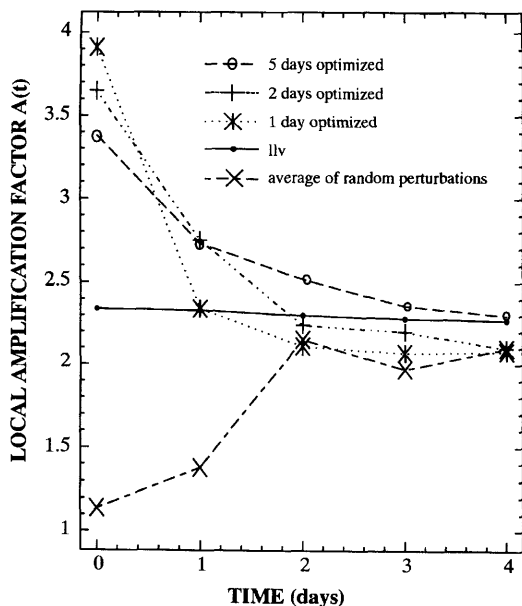


Fig. 13. Amplification factors for the first optimal vectors optimized for different long time periods. Also shown are the amplification factor associated with the estimated LLV and the local amplification factor averaged for fifteen initially random perturbations for the period 95–100 days in the nonlinear model integration.

but they quickly drop below the Lyapunov growth rate. The 5-day optimized optimal vector grows considerably faster than the Lyapunov vector only during the first day, after which its growth rate quickly converges to the Lyapunov exponent. Random perturbations start at a growth rate much lower than the Lyapunov rate, but after only two days they have an average instantaneous growth rate equal to or larger than the leading 24-hour optimal perturbation. This clearly shows that for a period longer than the optimization period, even a random perturbation may have a larger amplification factor than the leading optimal vector, since the latter may not project well on the leading instabilities of the system given by the local Lyapunov vector.

4. Summary

In this paper we first gave an overview of the definition of local Lyapunov vectors (LLVs) and optimal (or singular) vectors. We emphasized that

since all perturbations turn toward the leading LLV, it represents the fastest possible growth over a long time period leading to t_0 , while the optimal vector is the perturbation that maximizes growth for a finite time period, starting at t_0 .

The main results of this study pertain to the comparison of the leading LLV and the optimal vectors in a highly truncated (T10, 18 levels) version of the National Centers for Environmental Prediction Medium Range Forecast model. The major difference between the leading optimal vector defined by the total energy norm and the LLV is in their vertical structure. This difference (unlike the difference in the horizontal structure that was also found for short optimization periods) diminishes by the end of the optimization period. In fact, the initial optimal vectors are largely out of balance so the sudden changes in their vertical structure are associated with the geostrophic adjustment process.

At the initial time the leading optimal vectors with relatively long optimization period exhibit a growth rate significantly higher than that of the LLV. This extra, “super-Lyapunov” growth rate is due to the difference between the initial optimal vector and the LLV. By the end of the period of optimization, however, the growth rate associated with the leading optimal vector drops to the level of the Lyapunov exponent, as could be expected from the drastic changes in structure towards the LLV. The SVs optimized for 3-days or longer periods gain their growth from the combination of initial imbalance and baroclinic instabilities. The initial patterns are organized in such a way that by the time the geostrophic adjustment process takes place, the perturbations, just like the LLV, represent baroclinic instabilities.

Thus the optimization procedure can call upon two sources of error growth: (1) The rotation of the initial optimal vector toward the LLV (in this particular case, the geostrophic adjustment) and (2) the actual instantaneous growth along the components of the optimal vector along the leading LLVs (in this particular case, baroclinic instability). Apart from the rotation of the initial vector in the phase space, the largest possible growth is associated with the leading LLV. We found that for short (1–2 days) optimization periods the rotation associated with geostrophic adjustment is especially critical since the optimal vector at final time is still not along the vector providing

the fastest sustainable growth (first LLV.) These optimal vectors have a growth rate beyond the optimization period, which is below that associated with random perturbations. This may have adverse effects if optimal vectors with short optimization periods are used as initial perturbations for medium-range ensemble forecasts. In case of optimization for 3 days or longer periods, however, the optimal vectors at final time are close to the leading LLVs and thus provide close to the largest possible growth beyond optimization time.

It was also found that it takes three to four days for random perturbations to assume a direction (and associated amplification factor) close to that of the LLV. This time range corresponds well with the optimization period beyond which the initial optimal vectors become insensitive to further increases in the optimization period. Note that this is the time scale of individual synoptic events. This indicates that the optimal vectors, as compared to the LLV, provide a one-time-only extra perturbation growth that can be effective no longer than the life cycle of the most unstable phenomenon in the system, a baroclinically unstable synoptic event.

Our results confirm earlier findings that the optimal vectors are specific features that strongly depend on the norm and optimization time period chosen. In contrast, the leading local Lyapunov vector is independent of the choice of norm or any other tunable parameter; hence it is a basic and very general characteristic of the flow. This is reflected in the fact that all possible random linear perturbations in a system, including the optimal vectors, will converge to the first LLV. In other words, the LLV acts as a magnet that attracts all random perturbations, while the structure of the optimal vectors is "repelling": they turn away from their initial direction very rapidly toward the leading LLVs. The question whether the initial optimal vectors can occur naturally in a perturbation system will be addressed in the final section.

5. Discussion

In this section we present arguments, based on the results of simple model experiments (including those made in the present study), which are relevant to the properties of the optimal and Lyapunov vectors. However, it is necessary to perform experi-

ments with more complex systems, to verify whether these arguments would hold in general.

5.1. Are the optimal vectors off the attractor?

It is often assumed that the optimal vectors are capable of producing super-Lyapunov growth during the optimization period between t_0 and t_1 because, due to their construction (see eq. (18)), they "know" about the future evolution of the flow. This also assumes that the LLVs at t_0 do not know about the future evolution and reflect only past instabilities. This idea is probably not valid since, as Legras and Vautard (1996) showed, the leading LLVs define the unstable manifold of a system, which has the most impact on the future evolution of the flow, while the SVs have a substantial projection on the stable manifold that is of less importance with respect to future evolution.

As we saw in Section 3, the optimal vectors provide the extra super-Lyapunov growth through a one-time-only phase-space rotation of the initial vector. Increasing the optimization period beyond three days does not change the optimal vectors substantially. Similarly, experiments with the Zebiak and Cane (1987) simple coupled ocean-atmosphere model (Xue et al., 1996) indicate that the initial 3 or 6-month optimal vectors show a surprising lack of dependence on either the phase of the El-Nino/Southern Oscillation (ENSO) or the season. The same vectors at final optimization time (which should be similar at this time to the LLVs of the system) do show a strong dependence on ENSO phase and season. Apparently in the Cane-Zebiak system, as in our T10 model, the optimal vectors gain their super-Lyapunov growth from their unusual initial vertical structure. These facts suggest that, at least in these two rather simple systems, the optimal vectors offer no extra growth beyond that coming from their initial rotation, and consequently they may not exploit realistic (i.e., physically plausible) instabilities other than those present in the LLVs.

Since the evolution of the atmosphere and realistic atmospheric models are irreversible, the fact that the definition of the optimal vectors involves the future states of the system and requires the use of the adjoint equation, may indicate the possibility that some of these structures are not realizable. By "realizable" we mean that they may not project on the subspace of the first D

Lyapunov vectors, where $D \ll \text{dof}$ is the information dimension of the system (Kaplan and Yorke, 1979), as compared to the total number of degrees of freedom (dof) in the phase space of the system. The trajectories on the attractor evolve in a D -dimensional subspace of the whole dof-dimensional phase space that contains the attractor. The optimal vectors would direct to points that lie within the *attractor basin* but not on the *attractor itself* (i.e., not on, or near to, possible trajectories). So optimal vectors would point into directions that cannot be realized naturally in the system without external forcing, but from where the system would rotate rapidly onto a nearby trajectory. The initial optimal vector would move primarily along a leading LLV and the rotation would provide the extra-Lyapunov growth. With a three variable Lorenz model, Anderson (1995) also found that by moving along the first LLV in the Lorenz system one finds other nearby trajectories, while moving along the first optimal vector one reaches areas that are void of trajectories. These void regions are within the basin of the attractor (i.e., the system, if forced there, would return to one of the closest trajectories) but are not areas that the system visits naturally, without external forcing.

The suggestion that super-Lyapunov growth may arise from perturbation structures which are not within the attractor is also in agreement with studies that demonstrate the occurrence of super-Lyapunov growth, generally preceded by fast decay, starting from random perturbations (Trevisan and Legnani, 1995; Nicolis et al., 1995). Since these experiments are carried out in simple dynamical systems with initial white noise perturbations, the perturbations sample strongly parts of the phase space never visited naturally by the system. By contrast, in our study we used well balanced random perturbations representative of realistic differences among possible states. With balanced, realistic random perturbations, we found no super-Lyapunov growth in either in the current work or in previous higher resolution experiments (TK93). In other words, it is possible that super-Lyapunov growth can be observed in experiments starting with possibly off-the-attractor perturbations, but not in an unforced system, with perturbations lying within the attractor.

We note again that the largest possible growth

on the attractor can be associated with leading LLVs other than the first one. By super-Lyapunov growth we mean growth rates that are above those associated with any of the leading LLVs. In fact, if the initial structure of the singular vectors would be limited to the unstable manifold (i. e., the leading LLVs), the first SV would point into the direction of the LLV with the largest local amplification and there would be no initial adjustment associated with off-attractor perturbations that apparently can give rise to super-Lyapunov growth through different mechanisms. We note in passing by that the determination of the fastest growth that can occur on the attractor is computationally much more efficient by computing the LLVs (Benettin et al., 1980; Wolf et al., 1985) or the nonlinearly bred vectors (1993) than by computing the singular vectors (Buizza et al., 1993).

In our T10 experiments the "non-physical" process responsible for the super-Lyapunov initial growth of the SVs is associated with geostrophic imbalance. Other types of initial adjustment was documented by Molteni et al. (1996). When enstrophy was used as a norm to define the singular vectors, energy from the very large scales was found to *cascade up* to synoptic scales and cause very large growth rates at initial time. On the other hand, when the total energy is used as a norm, just the opposite happens: initially, the energy is confined mainly to smaller scales from where it *cascades down* to the synoptic scales (see also Hartmann et al., 1995). These processes can also be explained by adjustment processes. It is well known that the spectral distribution of kinetic energy in the mid-troposphere tends to keep a quasi-two-dimensional equilibrium. The control parameter of this equilibrium is the square of the average wavenumber, which is defined by the ratio of the enstrophy and the rotational kinetic energy of the atmospheric level. This parameter, which constrains the rotational kinetic energy to the synoptic scales in the MRF models, does not change essentially with the introduction of small-amplitude perturbations. Hence, if perturbation energy is *introduced* at low or high wavenumbers, an efficient adjustment process, in which energy moves (up or down) to the synoptic scales, arises to recreate the quasi-two-dimensional nonlinear equilibrium (Pedlosky, 1987, p. 164–178). We can compare this adjustment process in a general sense

to the geostrophic adjustment process discussed earlier in this paper.

These studies suggest that, at least in simple systems, the optimal vectors found with commonly used norms may not be realizable in a dynamical system without some kind of forcing. We recall that the computation of the singular vectors is a mathematical procedure in which the largest growth is searched for with the use of the linear and adjoint models. In these computations there is no guarantee that the structures determined are on the attractor of the system (and hence physically meaningful). This could be insured only with the careful (and difficult) selection of a norm, which provides the only additional constraint on the computations. So care should be used when interpreting the singular vectors and their role in atmospheric dynamics.

However, in more complex systems, and in the real atmosphere, initial optimal vectors, with some *specific norms*, may still have a role through the impact of random forcing. (Which norms may be most appropriate to use is still an open question, though.) The quasi-geostrophic dynamics of the atmosphere are constantly forced by interactions with the lower boundary and by processes like convection, which can be considered as random forcing on the large scale flow. As suggested by Farrell (1990), it is quite possible that at the initial stages of perturbation growth, the optimal perturbations may play a role on different scales of motions. Also, truncation errors in a GCM may introduce relatively large errors in the smallest resolved scales, possibly fueling super-Lyapunov error growth rates at the very small scales. However, since the singular vectors turn toward the leading LLVs very rapidly, their influence may be limited and also difficult to document.

5.2. *The use of singular vectors in analysis and ensemble forecasting*

It is also important to assess whether optimal perturbations and/or Lyapunov vectors are present in the atmospheric analysis errors. This is because they are the fastest growing errors, hence an analysis procedure should attempt to eliminate or reduce them. If one assumes that the initial analysis errors are white noise, then, by definition, the forecast errors would be dominated by optimal vectors, at least in the initial stages, before they

turn into LLVs. However, for this assumption to be true, data assimilation systems should be perfectly efficient in removing the growing error structures that inevitably appear in the 6-h forecast used as background field. Due to the use of dynamical techniques in data assimilation, this is virtually impossible, even with advanced techniques. As Pires et al. (1996) showed, under ideal conditions, a 4-dimensional variational assimilation would produce analysis fields that at the end of the assimilation period (i.e., start of forecast period) contain errors projecting *only onto the unstable manifold*, that can be best described by the LLVs.

It is a common experience with less advanced optimal interpolation or 3-dimensional assimilation techniques that forecast errors with very similar (but case dependent) patterns are observed on 24 h, 36 h, 48 h, ... 72 h and even 5-day forecasts verifying at the same time, with increasing magnitudes. This confirms that growing error structures present in the analysis and carried along by the 6-h forecasts during the analysis cycle can at least partially survive many successive analyses. This observation supports the idea that a conventional 3-D variational or OI analysis cycle is, to some extent, similar to a breeding cycle (TK93), and therefore the analysis errors must contain finite amplitude leading LLV structures. KT94 also found experimentally that the difference between the analyses and observations contained significant projections onto the bred vectors (nonlinearly estimated LLVs), and that the projections were much smaller when bred vectors corresponding to a different day were used.

Ensemble forecasting is another area affected by the potential presence of optimal vs. Lyapunov vectors in the analysis errors. The initial perturbations that are introduced onto the control analysis should represent possible analysis errors (TK96). So when the initial optimal vectors are used in ensemble forecasting one has to insure that through the use of an appropriate norm, the initial analysis error covariance structure is taken into account. With norms that do not satisfy this criterion one can obtain initial ensemble perturbations that are growing fast (measured with the norm chosen) but are not representative of uncertainty in the analysis. For example, we know that to a large extent, the analysis error is geostrophically balanced. Therefore the singular vec-

tors computed in this study with the use of the total energy norm are not representative.

On the other hand, we saw in Section 3 that, in the general circulation model used in this study, the initial optimal vectors with long enough optimization period (three days or more) turn into the direction of the leading LLVs. So under certain conditions there may not be much difference between an ensemble based on LLVs and optimal vectors — at least after the optimization period ends and if the errors initially develop linearly. This conjecture is supported by Barkmeijer (1995) who, with a T21L18 QG model found that the forecast error covariance matrix in a limited geographical area is essentially independent of the initial constraints introduced as the analysis (initial) error covariance matrix. Similarly, in their simulated analysis/ensemble forecast experiments, Houtekamer and Derome (1995) found no appreciable difference between the performance of the bred ensemble (based on the leading LLVs) and an ensemble based on optimal vectors. In their study, however, they used a quasi-geostrophic model in which nonlinearities appeared only after 4 days or so, during which period the optimal vectors may have assumed the structure of the LLVs. Houtekamer and Derome (1995) also used some special constraints in the form of a norm penalizing departures from a quasi-barotropic perturbation structure assumed to correspond to the structure of analysis errors, that presumably made the initial optimal vectors more similar to the LLVs.

Our goal in the present study was to focus on the basic Lyapunov characteristics of the flow, and compare the first LLV to the top portion of the optimal vectors spectrum in an atmospheric general circulation model. Since the model we have used is severely truncated, we compared our results to those from other studies and found that they are, in several respect, in good qualitative agreement. Nevertheless, we plan to carry out a similar investigation with a higher resolution version of the NCEP global spectral model in a future study.

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7. Appendix

The state of balance of the LLVs and optimal vectors

The basic flow of the atmosphere (and of the MRF model) is one of quasi-geostrophic balance. However, because the fast growing perturbations are associated with the time changes of the flow, there is no guarantee that the perturbations will be in a geostrophic or thermal balance. In this Appendix we show that whereas the LLVs are somewhat out of balance, the initial optimal vectors defined by the total energy norm are very strongly out of balance, so that the initial super-Lyapunov growth is dominated by the geostrophic adjustment process.

In the following quantitative estimation of the state of balance we assume that geostrophic adjustment takes place on a time scale much smaller than that of the evolution of the basic flow, which is a fairly good approximation. It is important to determine not only the extent of the lack of balance of the perturbations, but also whether the mass field adjusts to the velocity field or vice versa.

The perturbation thermal balance equation for a signal level σ_k is

$$A_k = B_k, \quad A_k = \frac{\partial^2 \psi}{\partial \sigma \partial x} (\sigma_k),$$

$$B_k = \frac{R}{f} \left(-\frac{1}{\sigma} \frac{\partial T}{\partial x} + \frac{\partial T}{\partial \sigma} \frac{\partial \Pi}{\partial x} + \frac{\partial T_b}{\partial \sigma} \frac{\partial \pi}{\partial x} \right) (\sigma_k),$$

where ψ , T , and π is the perturbation streamfunction, temperature, and log of surface pressure, respectively, while T_b , and Π are the temperature and the log of surface pressure for the background flow.

If we allow at time t for an initial lack of balance of the perturbations due to the forcing from the background flow, and neglect the time change of the background flow over the adjustment period, we can assume that the adjustment process will result in an approximate balance after a short interval r_k :

$$A_k(t + r_k) \approx B_k(t),$$

that is

$$A_k(t) + \frac{\partial A_k}{\partial t} (t) r_k \approx B_k(t).$$

Let $c_k(t) = B_k(t)/A_k(t)$. In a state of balance, $c_k = 1$, so that this parameter indicates the extent to which the perturbations are out of balance. If there is no forcing then $\partial|A|/\partial t$ is positive for $c_k > 1$ and negative for $c_k < 1$. However, if $|A_k|$ or $|B_k|$ is increasing due to the forcing from the background flow the other quantity will simply follow it with a time shift r_k . In this case, the adjustment interval can be positive, indicating that the velocity fields adjust to the forced temperature fields, or negative, in which case the mass field adjusts to the forced vorticity.

The adjustment period can be estimated from

$$r_k = \frac{\int_{t_0}^{t_0 + T_a} (c_k(t) - 1) dt}{\ln(Q_k(t_0, T_a))}.$$

$Q_k(t_0, T_a) = A_k(t_0 + T_a)/A_k(t_0)$ represents the relative growth of the velocity field over a given time period T_a . If the perturbation is forced, e.g., $c_k < 1$ and $Q_k > 1$ ($\partial|A_k|/\partial t > 0$) at the same time the above formula gives the time average of the adjustment period for an arbitrarily long period T_a .

We have computed the zonal average of c_k and Q_k for both the LLVs and the optimal vectors at latitude 50°S. The ratio of c_k for the LLVs varies from 0.75 to 0.95 in the midtroposphere (levels 4 through 10). The typical value of Q_k is 5.4 over 24 h, and the adjustment period r_k is -2.5 h. These results indicate that the slowly varying background flow is continuously forcing the perturbation LLVs. The resulting lack of balance is about 5–25%, and the thermal fields adjust to the vorticity fields with a time scale of 2–3 h.

For the 1-day optimal vectors, we find that the balance ratio $c_k(t_0)$ is -0.5 at level 4, and from levels 5 through 9, the ratio is above 10 (the largest imbalance occurs at level 5 where $c_k(t_0) = 15.2$). After one day, the ratios converge down to the values typical for the Lyapunov vectors. The adjustment time scale r_k is in the beginning negative for level 4, but positive for the other levels. The changes in the vertical wind shear, given by Q_k , are much larger than the temperature changes (Q_k reaches a maximum value of 70.7 for the first 24 h). After one day, the values of these parameters converge to those reported for the LLVs. These results indicate that: (a) the 1-day optimal vectors are in an initially extremely unbalanced state; (b) the initial velocity fields are much smaller than would be required to balance the temperature fields, and following this observation, (c) for most of the troposphere the velocity adjusts geostrophically to the temperature perturbation. Both the forcing and the geostrophic adjustment increases the vertical windshear. These results support the conclusion that the initial super-Lyapunov growth of the optimal vectors is dominated by geostrophic adjustment.

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