Prediction of the Probable Errors of Predictions

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ABSTRACT

We propose here a method of "stochastic-dynamic" prediction that is computationally more efficient than integration of the full set of "second-moment" equations. This gain is achieved by omitting covariances between modes in different interacting triads, and by expressing intratriad covariances in terms of error variances, via the conditions for invariance of products of invariants. The resulting evolution equations for the error variances of all modal amplitudes constitute a closed system involving only those error variances.

To test the accuracy of this method, we have compared the predicted error variances with those calculated directly from an ensemble of 100 individual predictions, starting from an ensemble of 100 initial states containing random errors. These agree very well up to about the doubling time of total rms error, but later diverge as the effects of indirect interactions accumulate.

1. Introduction

It has long been recognized that a considerable part of the error of numerical predictions originates from errors in specifying the initial state. The latter is reconstructed from a finite sample of widely scattered observations and is thus subject to nonsystematic instrument error, random roundoff errors in the transmitted data, and sizeable errors of interpolation. Accordingly, even if the reconstructed initial state were the *most probable* one, it should be realized from the outset that there are many neighboring initial states that are only slightly less probable. From this standpoint, it is only realistic to characterize the initial state by probability distributions of the discrete variables that describe a single state, rather than by the "most probable" values of those variables.

The strictly deterministic view of prediction tacitly presumes that a prediction originating in the most probable initial state inevitably leads to the most probable future state. Although this assumption is certainly justifiable for short periods, it is only an article of faith until one examines an ensemble of predictions originating in a large ensemble of initial states, drawn at random from a population whose probability distribution reflects the probability of error.

An even more important question concerns the behavior of the probability distribution of predicted states evolving from a large ensemble of neighboring initial states. If, for example, the probability distribution becomes more and more "spread out," an increasingly broad range of predicted states becomes almost as probable as the most probable state. Eventually, of course, all predicted states would become equally probable, so that prediction would be no better than guessing. Thus, a question that is of some present concern, and one that will become increasingly important as the range of predictions is extended, is the following: How does the "spread" or variance of an ensemble of predictions evolve from the variance of an ensemble of randomly chosen initial states? Does the variance grow with increasing range and, if so, on what does the rate of growth depend? The answers to these questions clearly have a direct bearing on such practical matters as the range beyond which predictions have no economic value, and on how much faith should be put in predictions of shorter range.

This brief outline of the nature of the problem is not intended to suggest that it is new. Some aspects of the problem concern the general question of predictability or overall growth of error, which has been studied from a theoretical standpoint by Thompson (1957), Novikov (1959), Lorenz (1965), Leith (1971) and Leith and Kraichnan (1972). Numerical experiments to investigate the gradual divergence of predictions from almost identical initial states have been carried out by Smagorinsky (1969), Lilly (1972), Herring *et al.* (1973), Daley (1981), Basdevant *et al.* (1981) and Vallis (1983). The most general of these studies, however, have dealt only with the dependence of error growth on the statistical properties of "true" or most probable states, such as the average kinetic energy spectrum, average static stability, and so on,

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rather than with the ways in which the errors evolve in specific situations and locales.

The present study, while it has obvious connections with the question of predictability, is more nearly directed toward the problem of "stochastic–dynamic" prediction, as stated by Epstein (1969). That work, whose aims were substantially those stated earlier in this introduction, was later extended by Fleming (1971) and Pitcher (1977). Briefly, both of the latter proposed to calculate the evolution of the first and second moments of the probability distribution of each modal amplitude in a spectral representation of the prediction model. Pitcher (1977), following Epstein (1969), integrated the moment equations with second-moment closure, while Fleming (1971) made calculations based on third-moment discard (second-moment closure), third-moment closure with the quasi-normal approximation, and third-moment closure with the "eddy-damped" quasi-normal approximation. The latter, in particular, predicts error variances that agree remarkably well with those calculated directly from an ensemble of individual predictions originating in an ensemble of neighboring initial states with prescribed variance. Fleming remarked that the volume of computation is "monumental, but finite"; Pitcher merely said that it is "excessive." In short, although their basic approach is extremely promising, its application in practice requires far more computation than does a single "deterministic" prediction.

The complexity of the moment equations arises from the nonlinearity of the original hydrodynamical equations. For even the simplest N-mode spectral models (e.g., two-dimensional nondivergent flow) the closed system of second-moment evolution equations with second-moment closure involves the variances of all N modal amplitudes, but potentially involves $N(N-1)/2$ covariances of pairs of modal amplitudes. Thus the complete system of second-moment equations consists potentially of $N(N+1)/2$ first-order ordinary differential equations in $N(N+1)/2$ variances and covariances. Each of these equations gives the rate of change of one of the moments as a linear combination of many of the others. In a general way, it may be said that the number of simple operations required to integrate this system over one time step varies as N^4, multiplied by a small fraction (reflecting the fact that not all triads of modes interact). This estimate is to be compared with the number of similar operations required to advance a single deterministic prediction over one time step; this varies roughly as N^2, again multiplied by a small fraction. Thus, the ratio of computing times for "stochastic–dynamic" prediction and "deterministic" prediction is on the order of N^2, a figure that rapidly approaches unreasonable values as N is increased.

Since we wish to predict only the error variances of the N modal amplitudes, it is natural to ask if it is possible to do so without explicitly predicting the $N(N-1)/2$ covariances, perhaps with some loss of accuracy but at much less computational expense. Briefly, the purpose of this note is to investigate this question.

The prediction model we have chosen is the simplest of a class of models that might be termed "quasi-geostrophic" or "quasi-nondivergent" and one whose treatment is easily extended to other models of that class, namely, two-dimensional nondivergent flow. It will be found most convenient to deal with the model equations in their spectral form. We start by deriving the equations for the evolution of small departures from the "true" modal amplitudes that, for some period of time, are quasi-linear in those departures and lead to a second-moment closure of the second-moment equations.

We then analyze the behavior of the basic structural element of a multimode system, which is a triad of three interacting modes. In this case, it is found possible to express the covariances exactly in terms of the error variances of the three modal amplitudes, owing to conservation of energy and enstrophy. Thus the evolution equations for the error variances of the three modal amplitudes constitute a closed system involving only the three error variances.

In the third section, we consider a five-mode system, consisting of two interacting triads with one mode in common, in order to investigate the effects of covariances of two different types. One type reflects indirect interactions between nonconnecting modes in different triads: our hypothesis is that these interactions remain weak throughout the early stages of error evolution. The other type is due to direct, intratriad interactions. As in the case of a single triad, it is found that the invariants of the five-mode system enable us to express the intratriad covariances in terms of the variances. Thus the evolution equations for the error variances of the five modal amplitudes form a closed system.

The third section is concluded with a discussion of the directions in which these methods can be extended to many-mode systems. In general, they lead to closed systems of N evolution equations for the error variances of N modal amplitudes. Thus the computation required to integrate these equations is comparable to that needed to complete a single deterministic prediction.

The fourth section is a description of some numerical experiments with a five-mode system, designed to test the hypothesis underlying the proposed methods. Approximate error variances are compared with those calculated directly from a large ensemble of individual predictions originating in a random ensemble of neighboring initial states with known variances.

The main results and conclusions are summarized in the fifth section.

2. The three-mode system

We shall first consider the spectral form of the vorticity equation for two-dimensional nondivergent flow. In the notation of Thompson (1972), in which the spectral equations are derived, it is

$$\frac{dA_k}{dt} = \sum_{i=1}^{N}\sum_{j=1}^{N} \beta_{ijk}\alpha_j^2 A_i A_j \quad (k = 1, 2, 3, \cdots, N), \quad (1)$$

where A_k is the streamfunction amplitude of the kth mode, multiplied by the corresponding eigenvalue α_k. The nonlinear interaction coefficients β_{ijk} are given by

$$\beta_{ijk} = -\frac{1}{\alpha_i\alpha_j\alpha_k}\int_A \phi_k J(\phi_i, \phi_j)dA. \quad (2)$$

Here the kth eigenfunction ϕ_k is the solution of $\nabla^2\phi_k = -\alpha_k^2\phi_k$, subject to the condition that ϕ_k either vanishes on the boundary of some closed domain A or satisfies periodicity conditions on the boundaries of A. The integral in (2) extends over the area A. Through integrating by parts and imposing the boundary conditions, it is readily shown that β_{ijk} vanishes if any two indices are equal, remains unchanged under cyclic permutation of indices, and reverses sign under noncyclic permutation.

In the simplest nontrivial case, when $N = 3$ Eq. (1) takes the form

$$\frac{dA_1}{dt} = \beta_{123}(\alpha_2^2 - \alpha_3^2)A_2A_3, \quad (3a)$$

$$\frac{dA_2}{dt} = \beta_{123}(\alpha_3^2 - \alpha_1^2)A_1A_3, \quad (3b)$$

$$\frac{dA_3}{dt} = \beta_{123}(\alpha_1^2 - \alpha_2^2)A_1A_2. \quad (3c)$$

Let us suppose that A_{10}, A_{20} and A_{30} are the most probable initial values of A_1, A_2 and A_3, and that $(A_{10} + A'_{10})$, $(A_{20} + A'_{20})$ and $(A_{30} + A'_{30})$ are slightly different initial values, each with a known (and somewhat lower) probability of being correct. We denote the deviations from A_1, A_2 and A_3 at later times by A'_1, A'_2 and A'_3. Thus, if we confine attention to the period of time during which $|A'_1| \ll |A_1|$, $|A'_2| \ll |A_2|$ and $|A'_3| \ll |A_3|$, the evolution equations for A'_1, A'_2 and A'_3 are given by (3a)–(3c) as

$$\frac{dA'_1}{dt} = \beta_{123}(\alpha_2^2 - \alpha_3^2)(A_2A'_3 + A_3A'_2), \quad (4a)$$

$$\frac{dA'_2}{dt} = \beta_{123}(\alpha_3^2 - \alpha_1^2)(A_1A'_3 + A_3A'_1), \quad (4b)$$

$$\frac{dA'_3}{dt} = \beta_{123}(\alpha_1^2 - \alpha_2^2)(A_1A'_2 + A_2A'_1). \quad (4c)$$

These are the basic evolution equations for the deviations from A_1, A_2 and A_3, originating in a single member of an ensemble of initial states neighboring A_{10}, A_{20} and A_{30}.

The usual evolution equations for the variances of A'_1, A'_2 and A'_3 are formed by multiplying (4a), (4b) and (4c) by A'_1, A'_2 and A'_3, respectively, and averaging over the ensemble. Thus, denoting the ensemble average by angle brackets, we see that

$$\frac{1}{2}\frac{d}{dt}\langle A'^2_1\rangle = \beta_{123}(\alpha_2^2 - \alpha_3^2) \times (A_2\langle A'_1A'_3\rangle + A_3\langle A'_1A'_2\rangle), \quad (5a)$$

$$\frac{1}{2}\frac{d}{dt}\langle A'^2_2\rangle = \beta_{123}(\alpha_3^2 - \alpha_1^2) \times (A_1\langle A'_2A'_3\rangle + A_3\langle A'_1A'_2\rangle), \quad (5b)$$

$$\frac{1}{2}\frac{d}{dt}\langle A'^2_3\rangle = \beta_{123}(\alpha_1^2 - \alpha_2^2) \times (A_1\langle A'_2A'_3\rangle + A_2\langle A'_1A'_3\rangle). \quad (5c)$$

That is, the changes in the variances of A'_1, A'_2 and A'_3 depend on the covariances $\langle A'_1A'_2\rangle$, $\langle A'_1A'_3\rangle$ and $\langle A'_2A'_3\rangle$. Initially those covariances vanish, simply because the ensemble of initial deviations A'_{10}, A'_{20} and A'_{30} is drawn at random from a population in which positive and negative values of equal magnitude are equally probable. At later times the covariances must be predicted.

The evolution equation for $\langle A'_1A'_2\rangle$ is constructed by multiplying (4a) by A'_2 and (4b) by A'_1, adding these equations, and taking the ensemble average. The result is

$$\frac{d}{dt}\langle A'_1A'_2\rangle = \beta_{123}(\alpha_2^2 - \alpha_3^2)(A_2\langle A'_2A'_3\rangle + A_3\langle A'^2_2\rangle) + \beta_{123}(\alpha_3^2 - \alpha_1^2)(A_1\langle A'_1A'_3\rangle + A_3\langle A'^2_1\rangle). \quad (6a)$$

Similarly, we find that

$$\frac{d}{dt}\langle A'_1A'_3\rangle = \beta_{123}(\alpha_2^2 - \alpha_3^2)(A_2\langle A'^2_3\rangle + A_3\langle A'_2A'_3\rangle) + \beta_{123}(\alpha_1^2 - \alpha_2^2)(A_1\langle A'_1A'_2\rangle + A_2\langle A'^2_1\rangle), \quad (6b)$$

$$\frac{d}{dt}\langle A'_2A'_3\rangle = \beta_{123}(\alpha_3^2 - \alpha_1^2)(A_1\langle A'^2_3\rangle + A_3\langle A'_1A'_3\rangle) + \beta_{123}(\alpha_1^2 - \alpha_2^2)(A_1\langle A'^2_2\rangle + A_2\langle A'_1A'_2\rangle). \quad (6c)$$

Examining (5a)–(5c) and (6a)–(6c), we observe that they comprise a closed system of six linear ordinary differential equations involving only the six variables $\langle A'^2_1\rangle$, $\langle A'^2_2\rangle$, $\langle A'^2_3\rangle$, $\langle A'_1A'_2\rangle$, $\langle A'_1A'_3\rangle$ and $\langle A'_2A'_3\rangle$. With the initial values $\langle A'^2_1\rangle = \langle A'^2_{10}\rangle$, $\langle A'^2_2\rangle = \langle A'^2_{20}\rangle$, $\langle A'^2_3\rangle = \langle A'^2_{30}\rangle$, $\langle A'_1A'_2\rangle = 0$, $\langle A'_1A'_3\rangle = 0$ and $\langle A'_2A'_3\rangle = 0$, these six equations can be integrated to find $\langle A'^2_1\rangle$, $\langle A'^2_2\rangle$ and $\langle A'^2_3\rangle$ at any time. The coefficients A_1, A_2 and A_3 are obtained by integrating (3a)–(3b), starting with $A_1 = A_{10}$, $A_2 = A_{20}$ and A_3

$= A_{30}$; they may be either pre-calculated, or calculated in parallel with the second moments.

The scheme outlined above will be recognized as equivalent to the "third-moment discard" method of Epstein (1969) and Pitcher (1977). As pointed out by Fleming, it cannot be expected to be accurate for periods approaching the maximum range of predictability. It might, however, be expected to be fairly accurate until the percentage errors become large.

It is also possible to predict the error variances without explicitly predicting the covariances. Let us start by differentiating (5a)–(5c) with respect to time. Then, substituting the expressions given in (3a)–(3c) and (4a)–(4c) for the time derivatives of A_1, A_2, A_3, A_1', A_2' and A_3', we find that

$$\frac{1}{2}\frac{d^2}{dt^2}\langle A_1'^2\rangle = \beta_{123}^2(\alpha_2^2-\alpha_3^2)[(\alpha_2^2-\alpha_3^2)A_2^2\langle A_3'^2\rangle + (\alpha_2^2-\alpha_3^2)A_3^2\langle A_2'^2\rangle + (\alpha_1^2-\alpha_2^2)A_2^2\langle A_1'^2\rangle + (\alpha_3^2-\alpha_1^2)A_3^2\langle A_1'^2\rangle + 2(\alpha_1^2-\alpha_2^2)A_1A_2\langle A_1'A_2'\rangle + 2(\alpha_3^2-\alpha_1^2)A_1A_3\langle A_1'A_3'\rangle + 2(\alpha_2^2-\alpha_3^2)A_2A_3\langle A_2'A_3'\rangle], \quad (7a)$$

$$\frac{1}{2}\frac{d^2}{dt^2}\langle A_2'^2\rangle = \beta_{123}^2(\alpha_3^2-\alpha_1^2)[(\alpha_3^2-\alpha_1^2)A_1^2\langle A_3'^2\rangle + (\alpha_3^2-\alpha_1^2)A_3^2\langle A_1'^2\rangle + (\alpha_1^2-\alpha_2^2)A_1^2\langle A_2'^2\rangle + (\alpha_2^2-\alpha_3^2)A_3^2\langle A_2'^2\rangle + 2(\alpha_1^2-\alpha_2^2)A_1A_2\langle A_1'A_2'\rangle + 2(\alpha_3^2-\alpha_1^2)A_1A_3\langle A_1'A_3'\rangle + 2(\alpha_2^2-\alpha_3^2)A_2A_3\langle A_2'A_3'\rangle], \quad (7b)$$

$$\frac{1}{2}\frac{d^2}{dt^2}\langle A_3'^2\rangle = \beta_{123}^2(\alpha_1^2-\alpha_2^2)[(\alpha_1^2-\alpha_2^2)A_1^2\langle A_2'^2\rangle + (\alpha_1^2-\alpha_2^2)A_2^2\langle A_1'^2\rangle + (\alpha_3^2-\alpha_1^2)A_1^2\langle A_3'^2\rangle + (\alpha_2^2-\alpha_3^2)A_2^2\langle A_3'^2\rangle + 2(\alpha_1^2-\alpha_2^2)A_1A_2\langle A_1'A_2'\rangle + 2(\alpha_3^2-\alpha_1^2)A_1A_3\langle A_1'A_3'\rangle + 2(\alpha_2^2-\alpha_3^2)A_2A_3\langle A_2'A_3'\rangle]. \quad (7c)$$

Inspecting these equations, we see that prediction of the variances requires calculation of six expressions involving the variances, each of which appears in two equations. The covariances enter only as a single linear combination, which appears in all three equations.

We shall next show that the relevant linear combination of covariances

$$C = (\alpha_1^2-\alpha_2^2)A_1A_2\langle A_1'A_2'\rangle + (\alpha_3^2-\alpha_1^2)A_1A_3 \times \langle A_1'A_3'\rangle + (\alpha_2^2-\alpha_3^2)A_2A_3\langle A_2'A_3'\rangle \quad (8)$$

is expressible as a linear combination of the variances. Multiplying (3a)–(3c) and (4a)–(4c) by A_1', A_2', A_3', A_1, A_2 and A_3, respectively, and adding these equations together, we first observe that

$$\frac{d}{dt}(A_1A_1' + A_2A_2' + A_3A_3') = 0 \quad (9a)$$

and, similarly, that

$$\frac{d}{dt}(\alpha_1^2A_1A_1' + \alpha_2^2A_2A_2' + \alpha_3^2A_3A_3') = 0. \quad (9b)$$

That is, the invariants of the system are

$$K = A_1A_1' + A_2A_2' + A_3A_3', \quad (10a)$$

$$E = \alpha_1^2A_1A_1' + \alpha_2^2A_2A_2' + \alpha_3^2A_3A_3'. \quad (10b)$$

We may think of K as the "error energy" and E as the "error enstrophy." Noting that the covariances vanish initially, we then see that the ensemble-averaged equation $\langle K^2\rangle = \langle K_0^2\rangle$ can be written as

$$A_1A_2\langle A_1'A_2'\rangle + A_1A_3\langle A_1'A_3'\rangle + A_2A_3\langle A_2'A_3'\rangle = \frac{1}{2}[(A_{10}^2\langle A_{10}'^2\rangle - A_1^2\langle A_1'^2\rangle) + (A_{20}^2\langle A_{20}'^2\rangle - A_2^2\langle A_2'^2\rangle) + (A_{30}\langle A_{30}'^2\rangle - A_3^2\langle A_3'^2\rangle)] = Q_1. \quad (11a)$$

Similarly, since $E^2 = E_0^2$,

$$\alpha_1^2\alpha_2^2A_1A_2\langle A_1'A_2'\rangle + \alpha_1^2\alpha_3^2A_1A_3\langle A_1'A_3'\rangle + \alpha_2^2\alpha_3^2A_2A_3\langle A_2'A_3'\rangle = \frac{1}{2}[\alpha_1^4(A_{10}^2\langle A_{10}'^2\rangle - A_1^2\langle A_1'^2\rangle + \alpha_2^4(A_{20}^2\langle A_{20}'^2\rangle - A_2^2\langle A_2'^2\rangle) + \alpha_3^4(A_{30}^2\langle A_{30}'^2\rangle - A_3^2\langle A_3'^2\rangle)] = Q_2. \quad (11b)$$

Finally, since $KE = K_0E_0$,

$$(\alpha_1^2+\alpha_2^2)A_1A_2\langle A_1'A_2'\rangle + (\alpha_1^2+\alpha_3^2)A_1A_3\langle A_1'A_3'\rangle + (\alpha_2^2+\alpha_3^2)A_2A_3\langle A_2'A_3'\rangle = \alpha_1^2(A_{10}^2\langle A_{10}'^2\rangle - A_1^2\langle A_1'^2\rangle) + \alpha_2^2(A_{20}^2\langle A_{20}'^2\rangle - A_2^2\langle A_2'^2\rangle) + \alpha_3^2(A_{30}^2\langle A_{30}'^2\rangle - A_3^2\langle A_3'^2\rangle) = Q_3. \quad (11c)$$

Examining (11a)–(11c), we see that these three equations may be regarded as a simultaneous system of linear equations in which $A_1A_2\langle A_1'A_2'\rangle$, $A_1A_3\langle A_1'A_3'\rangle$ and $A_2A_3\langle A_2'A_3'\rangle$ are the unknowns, and Q_1, Q_2 and Q_3 are known. Solving this system and substituting the results into (8), we find that

$$C = \frac{(\alpha_3^2-\alpha_1^2)^2(\alpha_1^2-\alpha_2^2)^2}{\Delta}[A_{10}^2\langle A_{10}'^2\rangle - A_1^2\langle A_1'^2\rangle] + \frac{(\alpha_2^2-\alpha_3^2)^2(\alpha_1^2-\alpha_2^2)^2}{\Delta}[A_{20}^2\langle A_{20}'^2\rangle - A_2^2\langle A_2'^2\rangle] + \frac{(\alpha_3^2-\alpha_1^2)^2(\alpha_2^2-\alpha_3^2)^2}{\Delta}[A_{30}^2\langle A_{30}'^2\rangle - A_3^2\langle A_3'^2\rangle],$$

where Δ is the determinant of the system (11a)–(11c). It will be noted that C vanishes initially (as it should) and becomes appreciable only after the variances depart considerably from their initial values.

Introducing the expression above into (7a)–(7c), we now see that these equations comprise a closed system of evolution equations for the variances $\langle A_1'^2\rangle$, $\langle A_2'^2\rangle$ and $\langle A_3'^2\rangle$. The significance of this result is that it is not necessary to predict the covariances explicitly. Its possible computational advantages are not very apparent in the three-mode case, simply because the number of covariances between pairs of modal amplitudes is small. A proposed extension of this approach to higher-order systems is explored in the next section.

3. A five-mode system

To gain some insight into the interaction between triads, we next consider a five-mode system consisting of two triads with one mode in common. The evolution equations for the modal amplitudes are

$$\frac{dA_1}{dt} = \beta_{123}(\alpha_2{}^2 - \alpha_3{}^2)A_2A_3, \quad (12a)$$

$$\frac{dA_2}{dt} = \beta_{123}(\alpha_3{}^2 - \alpha_1{}^2)A_1A_3, \quad (12b)$$

$$\frac{dA_3}{dt} = \beta_{123}(\alpha_1{}^2 - \alpha_2{}^2)A_1A_2 + \beta_{345}(\alpha_4{}^2 - \alpha_5{}^2)A_4A_5, \quad (12c)$$

$$\frac{dA_4}{dt} = \beta_{345}(\alpha_5{}^2 - \alpha_3{}^2)A_3A_5, \quad (12d)$$

$$\frac{dA_5}{dt} = \beta_{345}(\alpha_3{}^2 - \alpha_4{}^2)A_3A_4, \quad (12e)$$

and the evolution equations for departures from A_1, A_2, A_3, A_4 and A_5 are

$$\frac{dA_1'}{dt} = \beta_{123}(\alpha_2{}^2 - \alpha_3{}^2)(A_2A_3' + A_3A_2'), \quad (13a)$$

$$\frac{dA_2'}{dt} = \beta_{123}(\alpha_3{}^2 - \alpha_1{}^2)(A_1A_3' + A_3A_1'), \quad (13b)$$

$$\frac{dA_3'}{dt} = \beta_{123}(\alpha_1{}^2 - \alpha_2{}^2)(A_1A_2' + A_2A_1') + \beta_{345}(\alpha_4{}^2 - \alpha_5{}^2)(A_4A_5' + A_5A_4'), \quad (13c)$$

$$\frac{dA_4'}{dt} = \beta_{345}(\alpha_5{}^2 - \alpha_3{}^2)(A_3A_5' + A_5A_3'), \quad (13d)$$

$$\frac{dA_5'}{dt} = \beta_{345}(\alpha_3{}^2 - \alpha_4{}^2)(A_3A_4' + A_4A_3'). \quad (13e)$$

From (13a)–(13e) we could proceed to form the evolution equations for the five variances of A_1', A_2', A_3', A_4' and A_5' and the ten covariances of pairs of those variables, as we did in deriving (5a)–(5c) and (6a)–(6c) in the previous section. The question, however, is this: Can we avoid predicting the covariances explicitly? I have not found a way to do so exactly, but the results of the previous section suggest an approximate method for taking into account the interactions that are dominant in "building up" covariances from their vanishing initial values.

Below we exhibit typical equations for the second time-derivatives of three of the variances: one for a nonconnecting mode in the triad (1, 2, 3), one for a nonconnecting mode in the triad (3, 4, 5), and the other for the connecting mode 3:

$$\frac{1}{2}\frac{d^2}{dt^2}\langle A_1'^2\rangle = \beta_{123}^2(\alpha_2{}^2 - \alpha_3{}^2)[(\alpha_2{}^2 - \alpha_3{}^2)A_2{}^2\langle A_3'^2\rangle + (\alpha_2{}^2 - \alpha_3{}^2)A_3{}^2\langle A_2'^2\rangle$$
$$+ (\alpha_1{}^2 - \alpha_2{}^2)A_2{}^2\langle A_1'^2\rangle + (\alpha_3{}^2 - \alpha_1{}^2)A_3{}^2\langle A_1'^2\rangle] + 2\beta_{123}^2(\alpha_2{}^2 - \alpha_3{}^2)[(\alpha_1{}^2 - \alpha_2{}^2)A_1A_2\langle A_1'A_2'\rangle$$
$$+ (\alpha_3{}^2 - \alpha_1{}^2)A_1A_3\langle A_1'A_3'\rangle + (\alpha_2{}^2 - \alpha_3{}^2)A_2A_3\langle A_2'A_3'\rangle] + \beta_{123}\beta_{345}(\alpha_2{}^2 - \alpha_3{}^2)(\alpha_4{}^2 - \alpha_5{}^2)[A_2A_4\langle A_1'A_5'\rangle$$
$$+ A_2A_5\langle A_1'A_4'\rangle + A_4A_5\langle A_1'A_2'\rangle], \quad (14a)$$

$$\frac{1}{2}\frac{d^2}{dt^2}\langle A_3'^2\rangle = \beta_{123}^2(\alpha_1{}^2-\alpha_2{}^2)[(\alpha_1{}^2-\alpha_2{}^2)A_1{}^2\langle A_2'^2\rangle$$
$$+ (\alpha_1{}^2-\alpha_2{}^2)A_2{}^2\langle A_1'^2\rangle + (\alpha_3{}^2-\alpha_1{}^2)A_1{}^2\langle A_3'^2\rangle + (\alpha_2{}^2-\alpha_3{}^2)A_2{}^2\langle A_3'^2\rangle]$$
$$+ 2\beta_{123}^2(\alpha_1{}^2-\alpha_2{}^2)[(\alpha_1{}^2-\alpha_2{}^2)A_1A_2\langle A_1'A_2'\rangle + (\alpha_3{}^2-\alpha_1{}^2)A_1A_3\langle A_1'A_3'\rangle + (\alpha_2{}^2-\alpha_3{}^2)A_2A_3\langle A_2'A_3'\rangle]$$
$$+ \beta_{123}\beta_{345}(\alpha_1{}^2-\alpha_2{}^2)(\alpha_4{}^2-\alpha_5{}^2)[A_1A_4\langle A_2'A_5'\rangle + A_1A_5\langle A_2'A_4'\rangle + A_2A_4\langle A_1'A_5'\rangle$$
$$+ A_2A_5\langle A_1'A_4'\rangle] + \beta_{345}^2(\alpha_4{}^2-\alpha_5{}^2)[(\alpha_4{}^2-\alpha_5{}^2)A_4{}^2\langle A_5'^2\rangle + (\alpha_4{}^2-\alpha_5{}^2)A_5{}^2\langle A_4'^2\rangle + (\alpha_3{}^2-\alpha_4{}^2)A_4{}^2\langle A_3'^2\rangle$$
$$+ (\alpha_5{}^2-\alpha_3{}^2)A_5{}^2\langle A_3'^2\rangle] + 2\beta_{345}^2(\alpha_4{}^2-\alpha_5{}^2)[(\alpha_3{}^2-\alpha_4{}^2)A_3A_4\langle A_3'A_4'\rangle + (\alpha_5{}^2-\alpha_3{}^2)A_3A_5\langle A_3'A_5'\rangle$$
$$+ (\alpha_4{}^2-\alpha_5{}^2)A_4A_5\langle A_4'A_5'\rangle] + \beta_{123}\beta_{345}(\alpha_1{}^2-\alpha_2{}^2)(\alpha_4{}^2-\alpha_5{}^2)[A_1A_4\langle A_2'A_5'\rangle + A_1A_5\langle A_2'A_4'\rangle$$
$$+ A_2A_4\langle A_1'A_5'\rangle + A_2A_5\langle A_1'A_4'\rangle], \quad (14b)$$

$$\frac{1}{2}\frac{d^2}{dt^2}\langle A_5'^2\rangle = \beta_{345}^2(\alpha_3{}^2-\alpha_4{}^2)[(\alpha_3{}^2-\alpha_4{}^2)A_3{}^2\langle A_4'^2\rangle$$
$$+ (\alpha_3{}^2-\alpha_4{}^2)A_4{}^2\langle A_3'^2\rangle + (\alpha_5{}^2-\alpha_3{}^2)A_3{}^2\langle A_5'^2\rangle + (\alpha_4{}^2-\alpha_5{}^2)A_4{}^2\langle A_5'^2\rangle]$$
$$+ 2\beta_{345}^2(\alpha_3{}^2-\alpha_4{}^2)[(\alpha_3{}^2-\alpha_4{}^2)A_3A_4\langle A_3'A_4'\rangle + (\alpha_5{}^2-\alpha_3{}^2)A_3A_5\langle A_3'A_5'\rangle + (\alpha_4{}^2-\alpha_5{}^2)A_4A_5\langle A_4'A_5'\rangle]$$
$$+ \beta_{123}\beta_{345}(\alpha_1{}^2-\alpha_2{}^2)(\alpha_3{}^2-\alpha_4{}^2)[A_1A_4\langle A_2'A_5'\rangle + A_2A_4\langle A_1'A_5'\rangle + A_1A_2\langle A_4'A_5'\rangle]. \quad (14c)$$

The expression for $\frac{1}{2}(d^2/dt^2)\langle A_2'^2\rangle$ can be obtained from (14a) by cyclic permutation of the indices 1, 2, 3; that is, $1 \rightarrow 2$, $2 \rightarrow 3$ and $3 \rightarrow 1$. Similarly, the expression for $\frac{1}{2}(d^2/dt^2)\langle A_4'^2\rangle$ is obtainable from (14c) by cyclic permutation of the indices 3, 4, 5.

Let us first examine (14b), whose right-hand side consists of six groups of terms set apart by brackets. Two groups, the first and fourth, involve the variances of A_1', A_2', A_3', A_4' and A_5'. These are the only terms that are nonzero initially, and produce an immediate interaction between the two triads; they are the dominant terms for a considerable period of time.

Two other groups of terms, the second and fifth, are linear combinations of covariances between modes in the same triad. These are both of the same form as the expression given in (8) and will later be approximated by linear combinations of variances.

Each of these particular combinations of intratriad covariances, it should be noted, appears in three equations. Thus, each can be calculated once, stored and reused; this reduces the volume of computation considerably.

The remaining groups of terms, the third and sixth, are distinguished by the fact that they involve covariances between nonconnecting modes in different triads. Those covariances *and their time-derivatives* vanish initially and can be built up only by indirect interaction between the nonconnecting modes, acting through the intermediary connecting mode. We suppose that these interactions remain weak over the range of validity of (13a)–(13e), and thus omit the third and sixth groups of terms entirely. The assumption that they are negligible will be investigated in the next section.

Returning to the second and fifth groups of terms in (14b), let us first note that "error energy" and "error enstrophy" are invariant. That is, multiplying (12a)–(12e) and (13a)–(13e) by A_1', A_2', A_3', A_4', A_5', A_1, A_2, A_3, A_4 and A_5, respectively, and adding these equations, gives

$$\frac{dK}{dt} = 0 \quad \text{and} \quad \frac{dE}{dt} = 0,$$

where

$$K = A_1A_1' + A_2A_2' + A_3A_3' + A_4A_4' + A_5A_5', \quad (15)$$

$$E = \alpha_1{}^2A_1A_1' + \alpha_2{}^2A_2A_2' + \alpha_3{}^2A_3A_3' + \alpha_4{}^2A_4A_4' + \alpha_5{}^2A_5A_5'. \quad (16)$$

Moreover, the five-mode system possesses a third symmetrical invariant that does not involve modes 1 and 5. To see this, we multiply (12b)–(12d) and (13b)–(13d) by

$$-(\alpha_5{}^2-\alpha_3{}^2)(\alpha_1{}^2-\alpha_2{}^2)A_2', \quad (\alpha_5{}^2-\alpha_3{}^2)(\alpha_3{}^2-\alpha_1{}^2)A_3' \quad \text{and} \quad -(\alpha_4{}^2-\alpha_5{}^2)(\alpha_3{}^2-\alpha_1{}^2)A_4',$$

$$-(\alpha_5{}^2-\alpha_3{}^2)(\alpha_1{}^2-\alpha_2{}^2)A_2, \quad (\alpha_5{}^2-\alpha_3{}^2)(\alpha_3{}^2-\alpha_1{}^2)A_3 \quad \text{and} \quad -(\alpha_4{}^2-\alpha_5{}^2)(\alpha_3{}^2-\alpha_1{}^2)A_4,$$

respectively, and add these equations. The result is

$$\frac{dQ}{dt} = 0,$$

where

$$Q = -(\alpha_5{}^2-\alpha_3{}^2)(\alpha_1{}^2-\alpha_2{}^2)A_2A_2' + (\alpha_5{}^2-\alpha_3{}^2) \times (\alpha_3{}^2-\alpha_1{}^2)A_3A_3' - (\alpha_4{}^2-\alpha_5{}^2)(\alpha_3{}^2-\alpha_1{}^2)A_4A_4'. \quad (17)$$

It is clear that the invariant Q is independent of K and E, since it does not involve the amplitudes of modes 1 and 5.

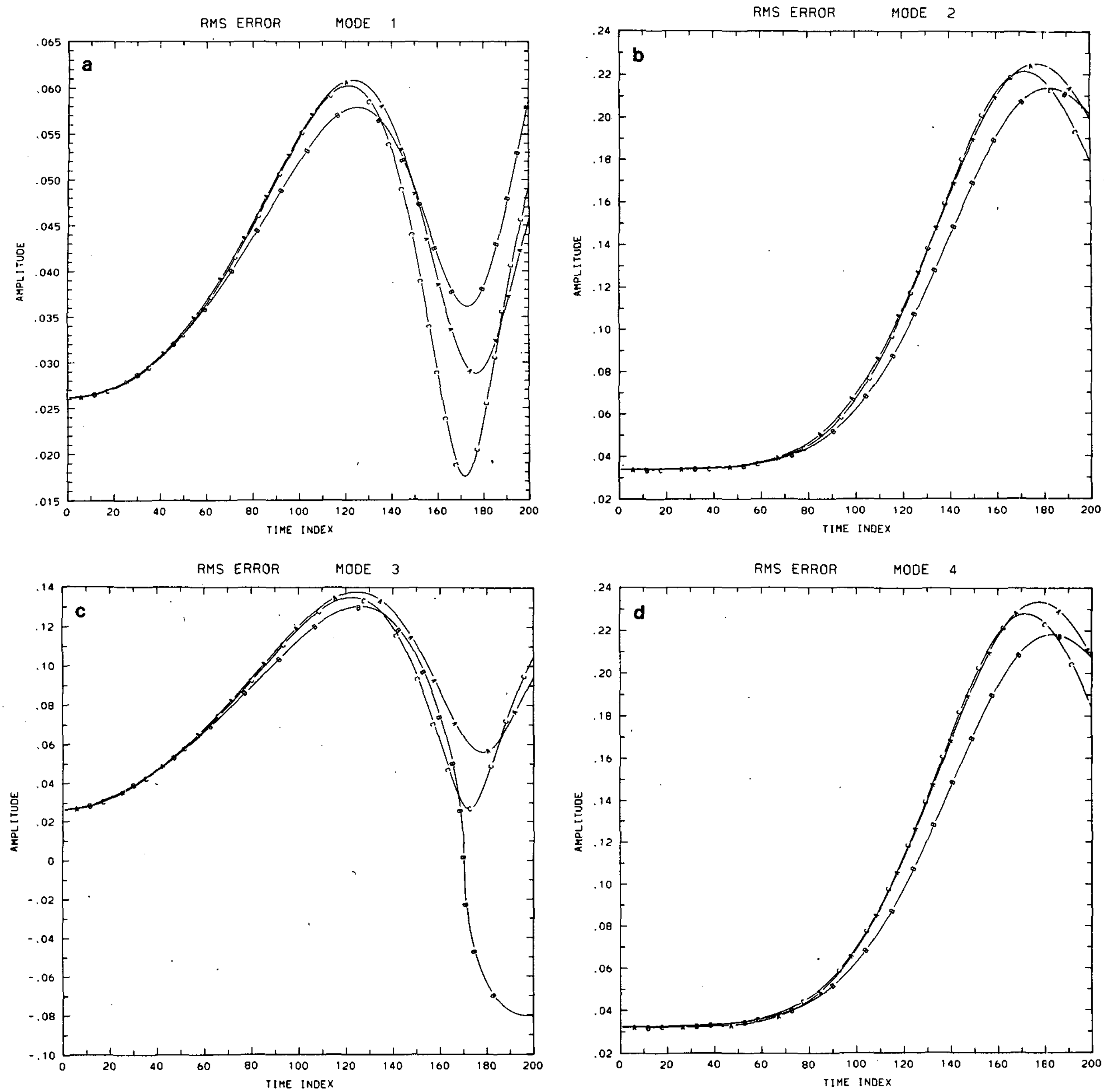

FIG. 1. Graphs of rms amplitude error plotted against time for: (a) mode 1; (b) mode 2; (c) mode 3; (d) mode 4; (e) mode 5 and (f) the total rms error. Curve A shows the results of the Monte Carlo calculations, while B and C give the results of the IID and SMC calculations, respectively.

The procedure for expressing the intratriad covariances in terms of the variances of A'_1, A'_2, A'_3, A'_4 and A'_5 is substantially that outlined in Section 2. We first express the fact that the products K^2, E^2, Q^2, KE, KQ and EQ, as given by (15), (16) and (17), are invariant, and average over the ensemble. Then, noting that all covariances vanish *initially* and omitting covariances between nonconnecting modes in different triads *at all times,* we write these six constraints as a simultaneous system of six linear equations in which the six unknowns are $A_1A_2\langle A'_1A'_2\rangle$, $A_1A_3\langle A'_1A'_3\rangle$, $A_2A_3\langle A'_2A'_3\rangle$, $A_3A_4\langle A'_3A'_4\rangle$, $A_3A_5 \times \langle A'_3A'_5\rangle$ and $A_4A_5\langle A'_4A'_5\rangle$. Finally, the solutions of this system, expressing each of these quantities as a linear combination of variances, are substituted in the second group of terms of (14a), the second and fifth groups of terms of (14b), and the second group of terms of (14c).

The result is that the equations for the second time-derivatives of the variances comprise a closed

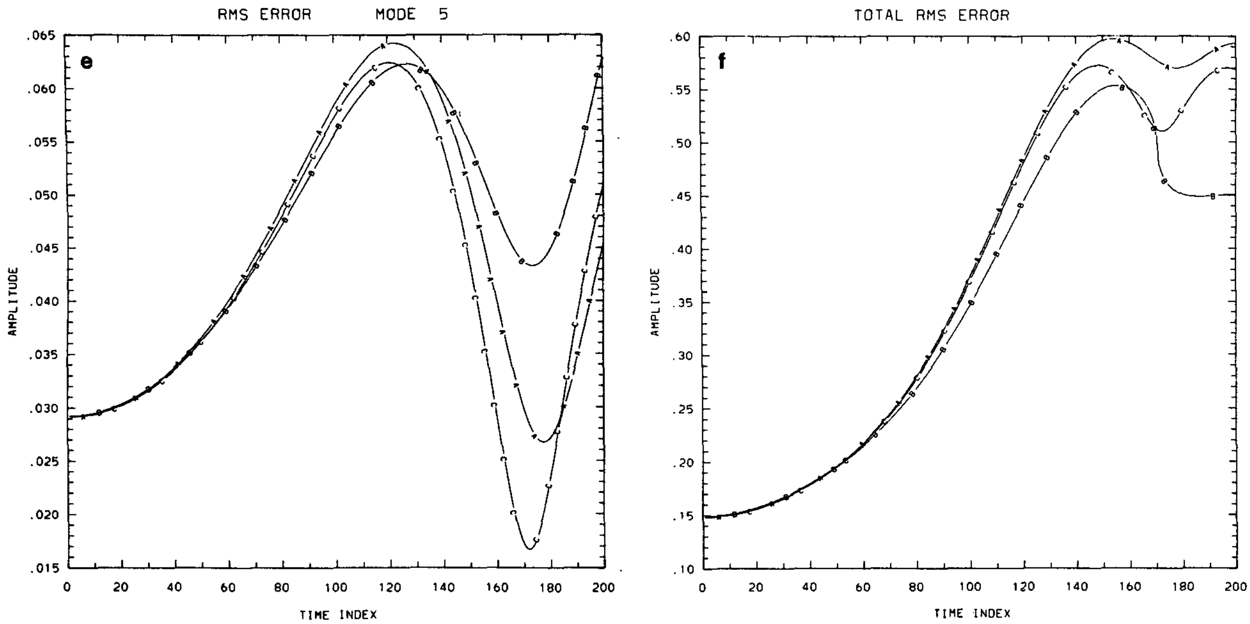

FIG. 1. (*Continued*)

system in the five variances. These are to be contrasted with the fifteen evolution equations for all second-order moments—five variances and ten covariances. The gain in computational efficiency is even more apparent as the number of modes is increased.

Before concluding this section, it should be noted that N-mode systems may be regarded as "chains" or branching "trees" of triads, connected by one or (more rarely) two common modes. If, for example, a $(2n + 1)$-mode system consists of an open "chain" of n triads, the equations for the second time-derivatives of the variances still have the same general form as (14a) and (14c) or (14b), and the same kind of approximation leads to a closed system of evolution equations for the $(2n + 1)$ variances. Such a system has at least $(n + 1)$ invariants, whereas the number of intratriad covariances is only $3n$. Thus, if we omit covariances between nonconnecting modes in different triads, the $\frac{1}{2}(n + 1)(n + 2)$ constraints of invariance of products of invariants are sufficient to express the intratriad covariances in terms of the variances.

We have made one crucial supposition about the behavior of the error covariances during the early stages of their evolution. Initially, of course, all covariances vanish. The initial time-derivatives of the intratriad covariance do not generally vanish, but the initial time-derivatives of the covariances between modes in different triads do vanish. Our supposition, then, is that the effect of indirect interactions through an intermediary connecting mode is negligible for a period that is long enough to establish the pattern and rate of error growth.

Our next concern, therefore, is to test this hypothesis. In the next section we show predictions of the variances of A'_1, A'_2, A'_3, A'_4 and A'_5 as calculated from the approximate equations for the second time-derivatives of the variances. These predictions are compared with integrations of the full second-moment equations with third-moment discard. Both of these approximate closures are then compared with the variances calculated directly from an ensemble of solutions of (12a)–(12e), starting from an ensemble of initial states neighboring a "most probable" initial state. In this way, we may see to what extent our suppositions about the covariances are correct, and (more fundamentally) the extent to which (13a)–(13e) are a valid description of the evolution of error.

4. Numerical tests of "indirect interaction discard"

To isolate the effects of two different types of approximations, we have predicted the error variances of the modal amplitudes in three different ways, but starting from the same ensemble of initial errors.

The ensemble of initial errors was generated by drawing 100 combinations of values of A'_{10}, A'_{20}, A'_{30}, A'_{40} and A'_{50} at random from a normally distributed population of errors, with known variance. Each of these combinations was then added to a single set of five hypothetically "true" or "most probable" initial values of A_{10}, A_{20}, A_{30}, A_{40} and A_{50}. The 100 combinations of error-contaminated initial values then define 100 initial states of the five-mode system discussed in Section 3.

The control experiment was a Monte Carlo calcu-

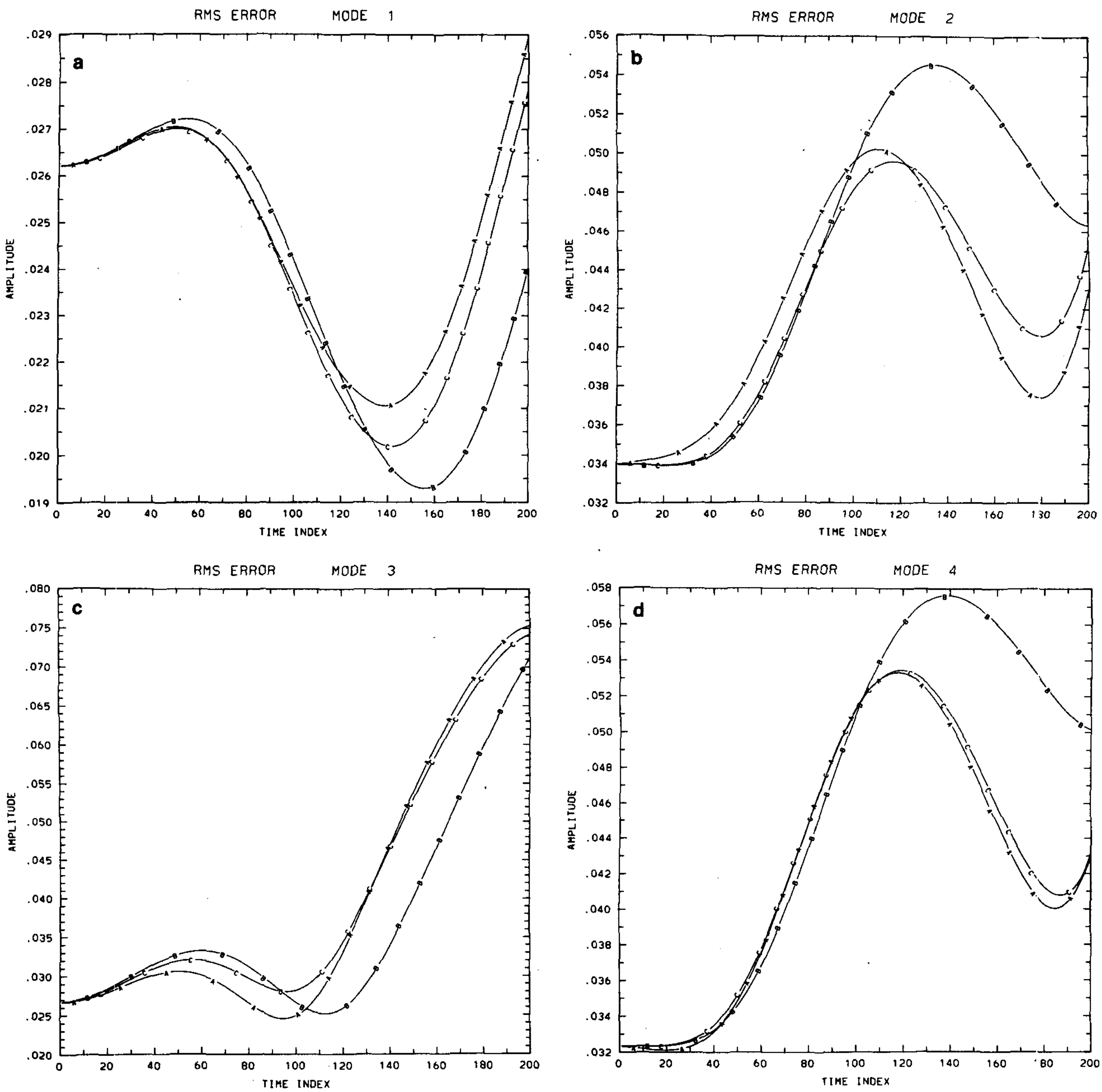

FIG. 2. As in Fig. 1 but for a different "true" initial state.

lation in which (12a)–(12e) were integrated 100 times, for each of the 100-member ensemble of error-contaminated initial states. The hypothetically correct values of A_1, A_2, A_3, A_4 and A_5 were predicted deterministically by integrating (12a)–(12e), starting from the "true" initial values A_{10}, A_{20}, A_{30}, A_{40} and A_{50}. The "correctly" predicted modal amplitudes were then subtracted from each of the 100 incorrect predictions, to obtain the ensemble of errors at each time stage. The ensemble error variance was calculated at each time stage, for each of the five modes separately and for all modes taken together.

The error variances predicted by the procedure described above are taken to be correct, i.e., representative of the error variances of an *infinite* ensemble. In this regard, a 30-member ensemble was found to be too small, in that the covariances of the initial errors were not invariably much smaller than their variances. The sampling error was reduced to tolerable proportions by increasing the sample size to 100.

A second method for predicting the error variances was simply to integrate the 15 evolution equations for the five error variances and ten covariances, as derived from (13a)–(13e), starting with the known initial error variances and setting the initial covariances to zero. This is essentially the method used by

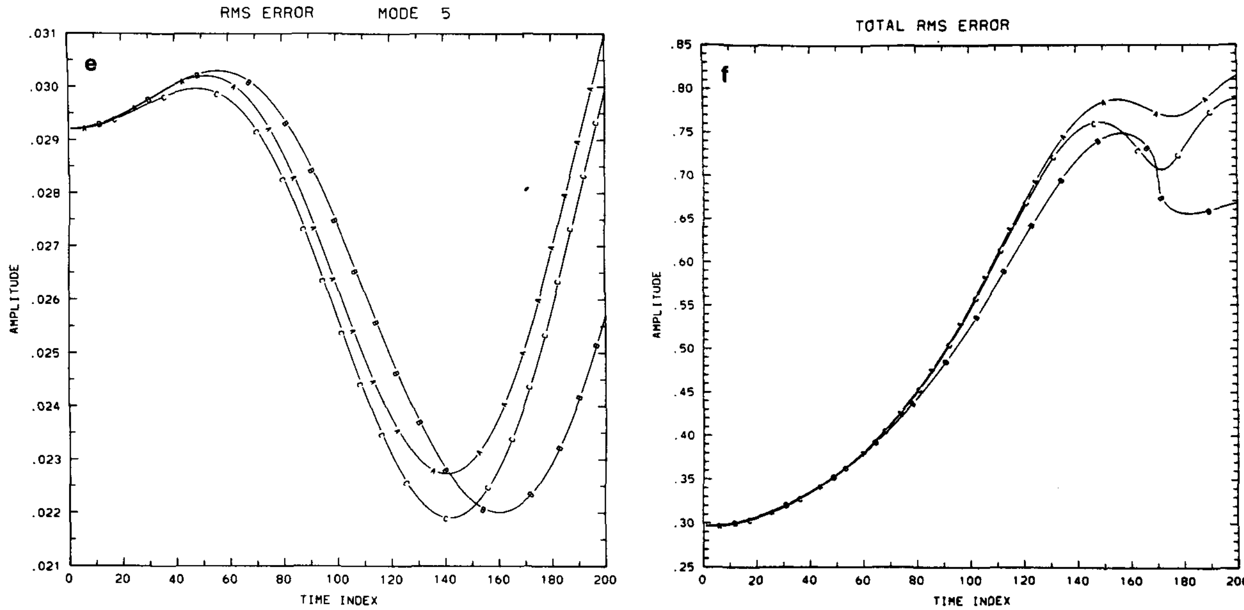

FIG. 2. (*Continued*)

Pitcher (1977). It gives results that differ from those of the Monte Carlo calculation, simply because third-order moments of the errors have been discarded. We refer to this method as SMC, for "second-moment closure."

The third method was to integrate the equations for the second time-derivatives of the error variances, as outlined in Section 3, discarding the covariances between nonconnecting modes in different triads and expressing the intratriad covariances in terms of the error variances. We refer to this method as IID, for "indirect interaction discard." Of the three methods considered here, it is computationally most efficient. It remains to be seen, however, what it sacrifices in the way of accuracy.

The three sets of calculations described above were repeated for three different situations, i.e., for three hypothetically "true" initial states, to see how the evolution of error variance is affected by different background conditions.

The results of these calculations are summarized in Figs. 1, 2 and 3, corresponding to three different "true" initial states. Each figure consists of six panels showing the root-mean-square error plotted against time; the first five panels show the rms error of the five modal amplitudes separately, and the sixth shows the total rms error. Each panel displays three curves. Curve A shows the rms error predicted by the Monte Carlo calculation, and curves B and C are the rms errors predicted by the IID and SMC methods, respectively.

In interpreting these results, the appearance of some important features can be anticipated. Since the covariances between modes in different triads and their first derivatives vanish initially, they vary as t^2 for small times t later than the initial time. Accordingly, it should be expected that the B and C curves should agree very well for "small" times, but diverge at "large" times. One of the main points of interest, then, is to see at what time the cumulative effects of discarded indirect interactions become large.

It should also be expected that the A curves (Monte Carlo calculation) and C curves (SMC method) would agree well as long as the errors remain small, but gradually diverge as the errors of third-moment discard accumulate.

Examining Figs. 1–3, we see that both the SMC and IID methods predict the rms error fairly well up to about 100 time units (roughly half the natural period of the five-mode system and about the doubling time of total rms error). In that range, the SMC method is accurate to within a few percent, and the IID method is generally accurate to within 10%. (Note that the numbering of the ordinate does not start with zero.) The latter result is accurate enough in this time range that the additional computational expense of the SMC method is probably not justified.

As anticipated, the IID and SMC calculations begin to diverge rapidly at 100–120 time units, about the time when the SMC and Monte Carlo calculations also begin to diverge. Exactly when this occurs depends on the "true" initial state, as can be seen by inspection of comparable graphs in different figures.

In any event, it appears that the "indirect interaction discard" method yields satisfactory predictions of rms error up to about the doubling time of total rms error. For the atmosphere, the doubling time is 2–3 days under average conditions. This range of values

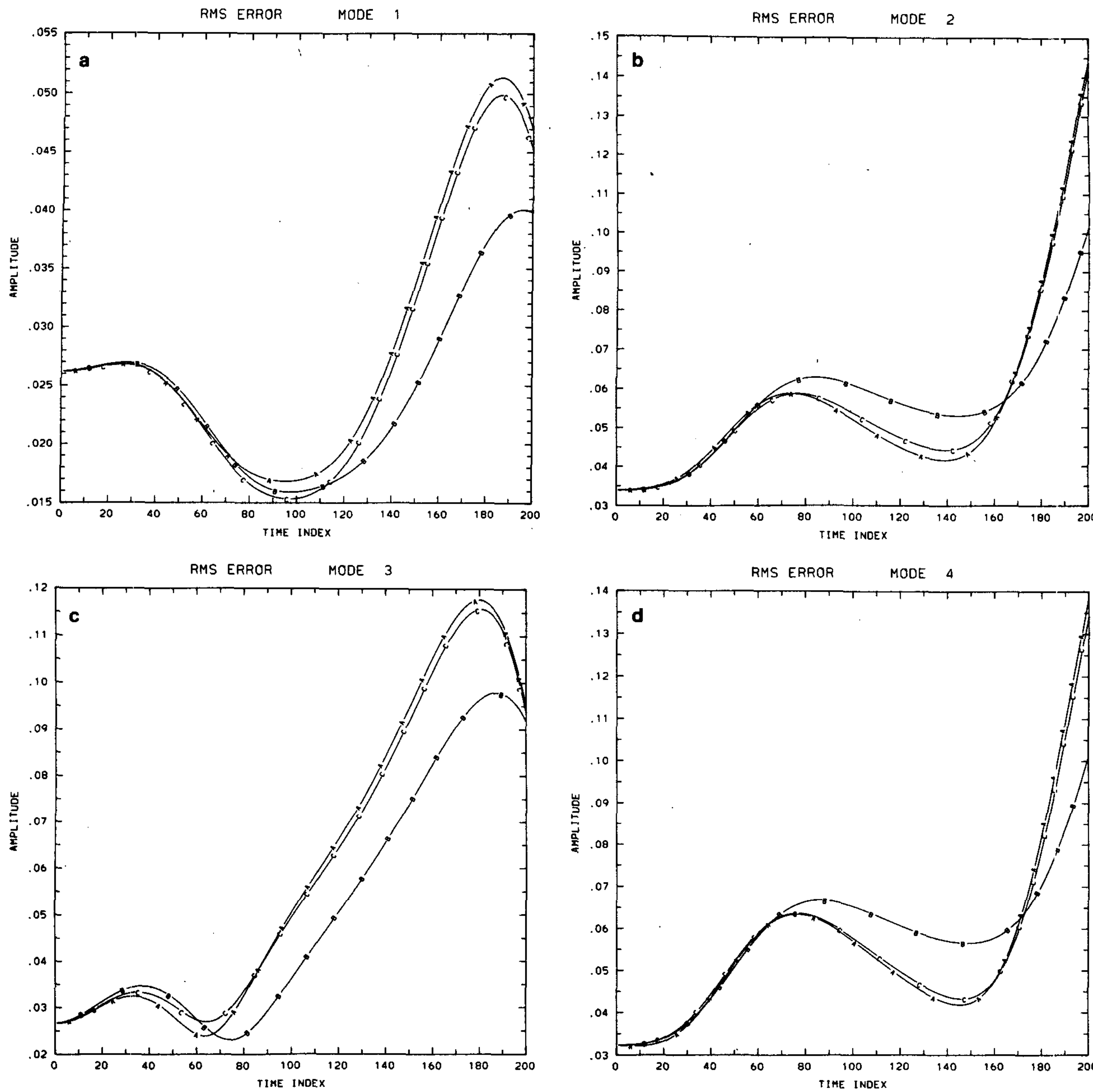

FIG. 3. As in Figs. 1 and 2 but for a third "true" initial state.

is supported by the theoretical and numerical studies of Thompson (1957), Novikov (1959), Lorenz (1969), Smagorinsky (1969), Leith and Kraichnan (1972) and Daley (1981).

The total rms error is predicted well by both the IID and SME methods up to about 140 time units, by which time the rms error has increased 2- to 4-fold.

5. Summary and conclusions

We have proposed a method of "stochastic–dynamic" prediction that is computationally more efficient than the "second-moment closure" or higher-order closures studied by Epstein (1969), Fleming (1971) and Pitcher (1977). This gain is effected partly by omitting covariances between nonconnecting modes in different triads. These covariances and their first time-derivatives vanish initially and can thus be expected to remain small for some short period of time. The remaining intratriad covariances are expressed in terms of variances by requiring invariance of products of the invariants of the system. As a result, the equations for the second time-derivatives of the error variances of all modes involve only those error variances and thus constitute a complete system.

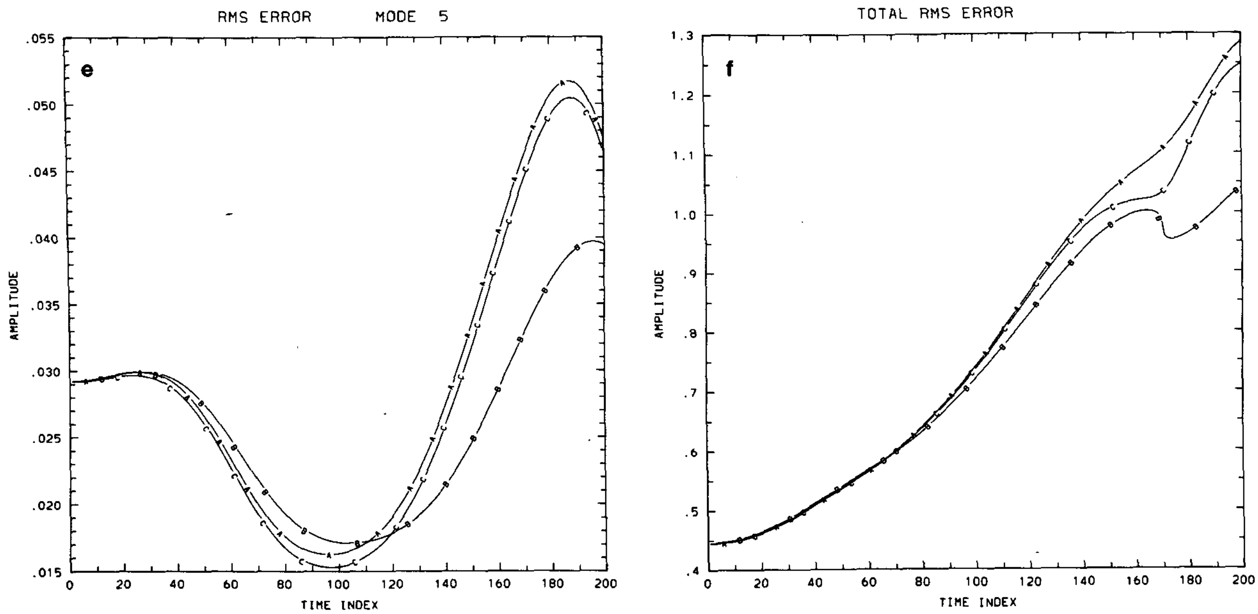

FIG. 3. (*Continued*)

This system is only slightly more complicated than the model equations for deterministic prediction.

The gain in efficiency is partially offset by a loss of accuracy at long times. Although the "indirect interaction discard" approximation is good at short times, it becomes cumulatively worse as the intertriad covariances build up. To test the accuracy of this method, we have carried out a series of numerical experiments with a five-mode system, consisting of two triads with one mode in common. Predictions of the modal error variances, based on both this method and the "second-moment closure," have been compared with those calculated directly from an ensemble of 100 predictions. The latter were generated from an ensemble of 100 neighboring initial states, whose errors were drawn at random from a normally distributed population with known variance. The comparisons show that the "indirect interaction discard" method predicts modal rms errors to within ~10% accuracy up to the doubling time of total rms error, which, for the atmosphere, is 2–3 days.

These results are promising, but any optimism should be tempered by the reminder that a five-mode system is a considerable idealization of the atmosphere. The next steps are clearly to apply the method to many-mode systems and to extend it to baroclinic models of the quasi-geostrophic or quasi-nondivergent type, which have invariants of the kind exploited here.

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