

What Is an Adjoint Model?



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ABSTRACT

Adjoint models are powerful tools for many studies that require an estimate of sensitivity of model output (e.g., a forecast) with respect to input. Actual fields of sensitivity are produced directly and efficiently, which can then be used in a variety of applications, including data assimilation, parameter estimation, stability analysis, and synoptic studies.

The use of adjoint models as tools for sensitivity analysis is described here using some simple mathematics. An example of sensitivity fields is presented along with a short description of adjoint applications. Limitations of the applications are discussed and some speculations about the future of adjoint models are offered.

1. Introduction

During the last 10 years the use of adjoints in meteorology has been rapidly increasing. Meteorologists working with adjoint models consider them exceptionally powerful modeling tools that will enable many outstanding problems to be solved efficiently and many old problems to be reexamined more directly. Three workshops [the first two reviewed by Errico et al. (1993a) and Prager et al. (1995), respectively] and a large portion of others have been devoted to the development and applications of adjoints. Still, many in the meteorological community are unaware of their existence or how useful they may be for the problems they are investigating.

Many questions investigated by research meteorologists concern sensitivity (e.g., Langland et al. 1995). Answering these questions requires estimating how much selected measured aspects of some synoptic features will change if perturbations are made to physical or dynamical processes or precursor synoptic con-

ditions. Once the “how much” is estimated, the question of “why” the change is as obtained can be more easily addressed by focusing on the significant aspects.

When quantitative estimates of sensitivity are desired, a mathematical model of the phenomena or relationships is required. Models have been used since their beginning to determine impacts of perturbations and thereby to estimate sensitivity. A more efficient, revealing, and direct way, however, is to use the model’s adjoint (Errico and Vukićević 1992; Rabier et al. 1992; Hall et al. 1982). The two methods, along with their limitations, will be contrasted in the next section.

Many meteorological questions also concern optimality. The best example is in data assimilation, where the *optimal* analysis is the one that fits all the observations best, consistent with what is known about the error characteristics of all the data used and assumptions made (Daley 1991; Lorenc 1986). For these applications, the adjoint is used as a tool for efficiently determining the optimal solutions (Lewis and Derber 1985; Tarantola 1987). Without this tool, the optimization problem could not be solved in a reasonable time for application to real-time forecasting.

Many other meteorological questions concern stability. These questions have often been answered by searching for exponentially growing, normal-mode solutions to some simply linearized model. Even when no such solutions are found, however, other types of

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growing solutions may still exist (Farrell 1988). Also, the linearized models previously used could not consider time-varying basic states, about which the linearization is performed. A more general method of stability analysis requires the use of an adjoint of the model (Farrell and Ioannou 1996a,b; Molteni and Palmer 1993). This generalized method includes the normal-mode method as a special case.

There are naturally limitations to the applicability of adjoint methods. Although one often does not find these discussed in the literature, they are related to limits of predictability and the chaotic nature of weather. The temporal range of applicability of adjoint-determined results remains very great, even more than many would expect, given that adjoints are based on a linearization of model equations (Errico et al. 1993b; R. Errico and K. Raeder 1997, manuscript submitted to *Quart. J. Roy. Meteor. Soc.*, hereafter ER).

The principal application of adjoint models is sensitivity analysis, and all its other applications may be considered as derived from it. This fundamental application will be described in sections 2–3, without recourse to mathematics beyond first-year calculus and first-semester linear algebra. Although adjoint models are often presented using mathematics unfamiliar to the great majority of meteorologists, the basic concepts are in fact very simple and likely familiar in other contexts. The few additional important details one obtains from consideration of higher-level mathematics can be easily learned once the basics are understood.

An example of an adjoint sensitivity calculation is described in section 4. Some applications of sensitivity analysis, including the contexts of stability analysis and optimization, are discussed in section 5. Limitations of the adjoint methods are described in section 6. Finally, the future development and application of adjoint models is discussed in section 7. They will likely become as common a tool as models themselves as the greater community of research and application meteorologists become aware of their power.

2. Sensitivity analysis

Adjoint operators can be derived for sets of equations that we do not normally call models, but since the examples to be used here apply to numerical weather forecast models, this presentation will invoke the term “model” with the understanding that this can be most sets of equations for most purposes [equations with terms whose first derivatives can be indetermi-

nate may require some special attention, e.g., Xu (1996)]. Furthermore, to keep the presentation simple, we will only consider numerical models that take a collection of numbers as input and produce another collection of numbers as output. Such a collection can be values of interior fields, boundary conditions, and model parameters defined in some discrete way, such as on a map grid or as spectral coefficients. This collection of input values can be simply denoted by a vector \mathbf{a} ; for example, the k th component of \mathbf{a} , which we denote as a_k , may be the temperature at some particular model grid point and pressure level at the model’s initial time. Similarly, the output at any time (or set of times) may be denoted by the single vector \mathbf{b} .

Often, interest in model solutions is focused on quantification of some output (forecast) aspects. Examples include mean-squared forecast errors, the central pressure predicted for a cyclone, the strength of a front measured in some way, or the total amount of rainfall predicted over some region and time. These measures of forecast aspects may be simply denoted as $J_n = J_n(\mathbf{b})$, where distinct n denote distinct measures. Although most applications of adjoint models that appear in the literature consider only J_n that are quadratic functions of the components of \mathbf{b} , the J_n need not be so restricted.

It is helpful to describe sensitivity analysis using adjoints by contrasting it with what has been called sensitivity analysis in most past literature in meteorology. In that literature a “control” solution (denoted here by subscript c) is determined by specifying \mathbf{a}_c , running the model to determine \mathbf{b}_c , and then computing a set of J_{nc} . A second solution is then determined by starting from some slightly altered \mathbf{a}_p to produce \mathbf{b}_p and J_{np} . The perturbation $\Delta\mathbf{a} = \mathbf{a}_p - \mathbf{a}_c$ must be sufficiently small (measured in some sense) that the case and model are not entirely altered so that any comparisons are meaningless. The results $\Delta J_n = J_{np} - J_{nc}$ are then used to describe the sensitivity of the model solution to perturbations of the kind introduced. From a single pair of control and perturbed forecasts, ΔJ_n can be computed for all J_n .

The problem with this previous type of sensitivity analysis is that, in fact, all that has been determined is the *impact* of one specific input perturbation $\Delta\mathbf{a}$ on the J_n . It is likely that another perturbation, having many of the characteristics and properties of the first perturbation (such as general location and root-mean-squared size), may yield very different ΔJ_n with correspondingly different interpretations of the sensitivity. This is especially true for short-term forecasts

where a few unstable modes of the solution may not have sufficient time to dominate the behavior of perturbations. In order to more generally answer the question of sensitivity using this method, an ensemble of perturbations must be examined (e.g., Mullen and Baumhefner 1994). Only then can it be claimed that, for example, “This J_n is more sensitive to wind perturbations here rather than there,” in place of just “This J_n is affected by this specific perturbation in this particular way.”

A very different approach to sensitivity analysis, with its own set of limitations, makes use of an adjoint of the model whose solution is being examined. As with the former method, it begins by considering a control solution \mathbf{a}_c . Next, it considers one selected J (from the set of J_n) and a corresponding vector of $\partial J/\partial \mathbf{b}$ evaluated at $\mathbf{b} = \mathbf{b}_c$, that is, the gradient of J with respect to possible perturbations of each component of the model output about the control solution. All that is required to determine this gradient is knowledge of the definition of J and that J be first-order differentiable with respect to the output components (e.g., specifications of each forecast field at each grid point) when J is evaluated for the control solution. This gradient can be interpreted as the sensitivity of J with respect to arbitrary (but small) perturbations of \mathbf{b} in the sense that

$$J' = \sum_k \frac{\partial J}{\partial b_k} \Delta b_k \quad (1)$$

is a first-order (Taylor series) approximation to ΔJ (primes will be used to denote linear estimates of perturbation quantities). For a Δb_k of a given magnitude, a large value of $\partial J/\partial b_k$ suggests that the perturbation will have a large effect on altering J , but a small value suggests the same perturbation will have a small effect.

An example J is the area-mean-squared surface temperature forecast error

$$J_T = \frac{\sum_{i,j} [T_{i,j}^{(f)} - T_{i,j}^{(v)}]^2 \Delta x_i \Delta y_j}{\sum_{i,j} \Delta x_i \Delta y_j}, \quad (2)$$

where the superscripts (f) and (v), respectively, denote forecast and verification values and the grid spacings in the x and y directions at the point i, j , respectively, are Δx_i and Δy_j . The corresponding gradient of J_T with respect to the forecast T evaluated about the control

forecast is

$$\frac{\partial J_T}{\partial T_{i,j}^{(f)}} = 2 \frac{[T_{i,j}^{(f)} - T_{i,j}^{(v)}] \Delta x_i \Delta y_j}{\sum_{i,j} \Delta x_i \Delta y_j}. \quad (3)$$

Knowledge of $\partial J/\partial \mathbf{b}$ reveals little we did not already know about the J , but what would reveal much more is knowledge of $\partial J/\partial \mathbf{a}$. This new gradient can also be interpreted as the sensitivity, but with respect to the initial conditions, boundary conditions, parameters, etc. (all the values that control the forecast and are included in the specification of \mathbf{a}). In particular,

$$J'_n = \sum_k \frac{\partial J_n}{\partial a_k} \Delta a_k \quad (4)$$

is also a (different) first-order approximation to ΔJ but does not require a forecast to determine $\Delta \mathbf{a}$. If one is interested in the impacts on J due to many different perturbations, one need simply compute the inner product (4) using the different Δa_k . The gradients of J with respect to either the input or output must be related since \mathbf{b} is determined by \mathbf{a} . In fact, what is required is a means to efficiently determine $\partial J/\partial \mathbf{a}$ from $\partial J/\partial \mathbf{b}$. The adjoint of the model is the tool used to do this.

3. Tangent linear and adjoint models

Since most of us are more accustomed to thinking in terms of integrating models forward in time rather than determining sensitivities backward in time, the adjoint of a model is most easily described by first discussing its corresponding tangent linear model. While it is not necessary to do so, the mathematics is significantly simplified by considering numerical models that are discretized in time (as almost all our numerical models are). Such a model may be simply described by

$$\mathbf{b} = B(\mathbf{a}), \quad (5)$$

where B denotes the model operator.

If \mathbf{a}' denotes an input perturbation, then

$$\Delta b_j \approx b'_j = \sum_k \frac{\partial b_j}{\partial a_k} a'_k \quad (6)$$

is a first-order Taylor series approximation to the resulting perturbation of the output that is valid as long as the $|a'_k|$ are all sufficiently small and the derivatives in (6) exist. Only for simple models can the analytical form of the derivatives in (6) actually be determined. Fortunately, for many of the most important applications, only numerical results are necessary; that is, numbers corresponding to the sums in (6) for each j are all that are required. Even they would be too inefficient to compute if all the derivatives of the output with respect to input, as written in (6), actually had to be explicitly numerically evaluated. Instead, it is often sufficient to determine only the net result of (6) by considering the model as a sequence of operations; for example,

$$B(\mathbf{a}) = B_N \left(\left(\dots \left\langle B_2 \left\{ B_1 \left[B_0(\mathbf{a}) \right] \right\} \right\rangle \dots \right) \right), \quad (7)$$

where the subscripts refer to individual time steps, iterations, and physical or algorithmic components of the model. The chain rule of elementary calculus can be applied to (7) to yield a sequential formulation for (6):

$$b'_j = b'_j{}^{(N)},$$

$$b'_j{}^{(n)} = \sum_k \frac{\partial b_j^{(n)}}{\partial b_k^{(n-1)}} b'_k{}^{(n-1)}, \quad \text{for } N \geq n \geq 1, \quad (8)$$

$$b'_j{}^{(0)} = \sum_k \frac{\partial b_j^{(0)}}{\partial a_k} a'_k,$$

where, for example, $b_j^{(n)}$ refers to the j th component of the output after step n . It is therefore possible to determine (6) using a sequence of simple and elementary calculations.

In specific numerical applications, the derivatives in (6) or (8) are to be evaluated at $\mathbf{a} = \mathbf{a}_c$ and the resulting sequence $\mathbf{b}^{(n)}$, so it is sufficient that they exist for only those particular values of the components of \mathbf{a} and $\mathbf{b}^{(n)}$ rather than for all possible values (i.e., the model operator must only be differentiable along the control trajectory). For spatially and temporally discrete models, this is often the case, even when the functions used in the model have discontinuities, as when modeling convection. The matrix that describes the set of derivatives appearing in (6) is called the Jacobian

of the model, determined with respect to model input. It is also called the linearized model operator (Kayo et al. 1997) or propagator, but here the term Jacobian will be used.

Equation (6) is linear in the perturbation quantities and is therefore a linearized version of the model. In meteorology's early days, such linearizations were performed about very idealized (control) solutions since the goal then was to eliminate enough terms and simplify all the others to obtain analytical solutions. As long as we are interested in numerical rather than analytical solutions, however, (6) need not be restricted to such idealized control solutions. In fact, (6) will likely become more accurate as we consider the \mathbf{a}_c that actually interest us because then relevant perturbations can truly become small relative to the control forecast values (e.g., contrast perturbed values of advective terms when a linearization is performed about a zonally uniform wind versus a real analyzed wind when the perturbations are intended to represent a possible difference between the true atmospheric state and the control state). The linearization can be performed about realistic model solutions that vary in all space directions as well as in time; that is, the reference solution need not be stationary. Such a model is called a tangent linear model, because the linearization is performed with respect to tangents of the model trajectory described in a model phase space.

For $J = J(\mathbf{b}) = J[B(\mathbf{a})]$, application of the chain rule of elementary calculus yields a linear relationship for gradients analogous to (6):

$$\frac{\partial J}{\partial a_j} = \sum_k \frac{\partial b_k}{\partial a_j} \frac{\partial J}{\partial b_k}. \quad (9)$$

There are three important differences between (6) and (9): (6) relates perturbations but (9) relates (sensitivity) gradients; (6) takes perturbations of the input to determine those for the output, but in (9) the roles of input and output are reversed; and the order of the subscripts j, k in (9) is reversed from those in (6). The reversal of subscripts in (9) indicates that the Jacobian matrix in (6) has been replaced by its transpose (i.e., the interchanging of rows and columns), or in more general mathematical terms by its adjoint. Equation (9) is therefore called the adjoint model corresponding to (6) [or, less precisely, (5)].

Note that the adjoint operates backward in the sense that it determines a gradient with respect to input from a gradient with respect to output. In a tem-

porally continuous model this would appear as an integration backward in time. Neither the model nor its tangent linear version is being integrated backward in (9), however, since it is the *adjoint* of the model equations that appears there. If there are no numerical instabilities associated with irreversible processes in the tangent linear model acting forward in time, there will be none in the adjoint acting backward in time.

The proper formulation of a tangent linear model requires simply that the Jacobian is properly computed and used so that (6) properly describes the behavior of perturbations as the perturbation size decreases toward zero. The usefulness of its results, however, depends on (6) being a good approximation to results obtained from differences between perturbed and controlled nonlinear solutions, since it is almost always the behavior of perturbations in the nonlinear model that actually interest us. The accuracy of this approximation will depend on the size of the input perturbation. Usually we are interested in perturbations that have the size of uncertainties in the input values, not infinitesimal values. The more nonlinear the model formulation and the closer solution trajectories come to critical points that determine conditionals in the model formulation, the smaller the acceptable size of perturbations will generally be. Experience with tangent linear versions of numerical weather prediction models suggests that they have much utility for perturbations the size of initial condition uncertainty on meso- α and larger scales, at least when the physics is dominated by dry dynamics. It is difficult to specify an accuracy that generally applies, since results greatly depend on details of the synoptic situation, perturbation size and structure, forecast duration, and forecast aspects of interest, as well as the intended application (Errico et al. 1993b; ER; Lacarra and Talagrand 1988).

The accuracy of an application of the adjoint model result to a finite-size perturbation is identical to that for the corresponding application of the tangent linear model in the specific sense that a J' computed from (1) by evolving a perturbation forward in time using the tangent linear model will be identical to that computed from (4) by evolving the gradient backward in time using the adjoint model. The gradient computed by the adjoint will be exact, however, only when the Jacobian is formulated and used properly without approximation. In most current adjoint models, approximations are made to the Jacobians (e.g., by neglecting some diabatic terms in the model) so that computed gradients are also only approximations. Their suitability will depend on the application.

4. Examples of adjoint fields

As an example of the output of an adjoint model, sensitivity fields like those shown in Errico et al. (1993b) are presented here. The model used is version 2 of the Mesoscale Adjoint Modeling System (denoted as MAMS2) developed at the National Center for Atmospheric Research (NCAR; ER). It is based on an earlier version described by Errico et al. (1994), although the changes are numerous and significant.

MAMS2 is a limited-area, primitive equation model prescribed in flux form on an Arakawa B grid (Arakawa and Lamb 1977) with Lambert conformal mapping. Its lateral boundary conditions are formulated using a Davies and Turner (1977) relaxation scheme applied within five grid points of the edge using a relaxation coefficient that exponentially decreases inward from the grid's edge. The time scheme is split-explicit following Madala (1981) with an Asselin (1972) time filter. It includes an adiabatic vertical mode initialization scheme (Bourke and McGregor 1983) of the external and first internal modes.

The model's vertical coordinate is $\sigma = (p - p_t)/(p - p_s)$, where p is pressure, p_t is the model top at 1 kPa here, and p_s is surface pressure. In all the experiments here, the wind components (eastward u , northward v), temperature (T), and mixing ratio (q) are defined on 10 equally spaced levels in values of σ . The vertical finite differencing follows the energy-conserving formulation of the NCAR Community Climate Model (CCM version 2; Hack et al. 1993).

The model physics includes a stability-independent bulk formulation of the planetary boundary layer following Anthes et al. (1987) and a stability-dependent vertical diffusion following CCM version 3 (Kiehl et al. 1996) treated using an implicit temporal scheme. Horizontal diffusion is a fourth-order scheme with a time-independent coefficient $k_h = 1.73 \times 10^{15} \text{ m}^4 \text{ s}^{-1}$ applied to the wind, temperature, and water vapor (mixing ratio) except next to the boundaries where diffusion is second order. There is also a convective adjustment scheme that acts on temperature only, with no accompanying mixing of moisture. The prognostic equation for ground temperature includes radiative effects modeled identically to that in Anthes et al. (1987). Moist convection is modeled using the relaxed Arakawa-Schubert scheme developed by Moorthi and Suarez (1992). Nonconvective precipitation is simply an enthalpy-conserving adjustment back to 100% relative humidity.

The tangent linear and adjoint versions of MAMS2 are exact, meaning that all terms are linearized properly, except for two approximations. One concerns the frequency with which the linearization is performed along the control trajectory and has been shown to have negligible impact on accuracy for most important applications (Errico et al. 1993b; ER). The other is that for the moist and dry convective physics, the required Jacobians are computed by a perturbation method to approximate $\partial b_j^{(n)}/\partial b_k^{(n-1)}$ by $\Delta b_j^{(n)}/\Delta b_k^{(n-1)}$ for a small $\Delta b_k^{(n-1)}$. This approximation has also been shown to be sufficiently accurate for many applications and has several useful benefits in addition to enhanced computational efficiency (ER).

The synoptic case to be shown is one of explosive cyclogenesis covering the 24-h period starting 0000 UTC 14 February 1982. The model grid covers the domain shown in Fig. 1 with a horizontal grid spacing of approximately 120 km. The initial and boundary conditions are obtained from European Centre for Medium-Range Weather Forecasts analyses interpolated to the MAMS2 grid. The analyzed 50-kPa height at the initial time, the analyzed sea level pressure at both the initial and verification (final) time, and the 24-h accumulated forecast precipitation are presented in Figs. 1a–d. The forecast cyclone (not shown) has central pressure of 96.9 kPa and is positioned approximately 270 km to the southwest of the verifying one.

For a J of frequent interest, we have chosen the vertical component of relative vorticity at the final time averaged within the area shown in Fig. 1c and extending through the bottom half of the atmosphere. The gradient of this J with respect to the final-time v field on the $\sigma = 0.65$ surface is shown in Fig. 2a. Note that because the vorticity is being spatially averaged, J actually depends on the circulation (i.e., tangential wind, according to Stokes's theorem) along the perimeter of the box.

The gradient of J with respect to the initial conditions is determined by applying the adjoint of MAMS2 to the gradient of J with respect to the output (i.e., patterns identical to that in Fig. 2a for $\partial J/\partial v$ at the lowest five model levels and analogous, but 90° rotated, patterns for $\partial J/\partial u$). The resulting gradients for J with respect to the input v , T , and q on the $\sigma = 0.65$ surface are shown in Figs. 2b–d. This is the model level where the maximum values of components of the gradient with respect to each field are found. For proper interpretation, the presented gradient values are best weighted by the inverse of the mass in the corresponding grid box (otherwise large gradient values are fa-

vored in large grid boxes), but on this grid, all grid boxes have almost equal mass (departing only because the surface pressure varies) and no weighting has been applied. The physical dimensions of the units for the gradients are those of J (vorticity here) divided by those of the corresponding fields. The gradients shown are therefore distinct from the corresponding fields themselves. The time $t = 0$ on the sensitivity plots indicates the verification (end forecast) time and $t = -24$ h indicates the initial time for the forecast, illustrating that the adjoint operates backward in time. The gradient for this single J with respect to all fields and points was obtained with a single application of the adjoint.

The computed gradients have a simple direct interpretation as fields of "sensitivity." For example, the field of $\partial J/\partial v$ for the input (i.e., $t = -24$ h) indicates that a perturbation of v of 1 m s⁻¹ at $\sigma = 0.65$ at the single point where the sensitivity has maximum value over the Atlantic in Fig. 2b will change the forecast J by 0.9×10^{-8} s⁻¹ (obtained by multiplying the value of the perturbation by the corresponding value of the gradient). If, instead, a perturbation of T of 1 K is introduced at the point marked where it is a minimum in Fig. 2c, J will change by -8.7×10^{-8} s⁻¹. If both perturbations (or others) are introduced simultaneously, the net change is simply given by the sum of the separate changes (a consequence of the linearization). Since J is linear, if the perturbations are introduced in the tangent linear model, this estimate of ΔJ would be exact. If J depended nonlinearly on the model output or if the initial perturbation were introduced in the nonlinear model, the change in J determined by the sensitivity calculation would only be an estimate of the change obtained (but under many conditions, a highly accurate one).

The sensitivity fields do not alone indicate where initial condition errors are nor what is necessarily "important" in producing the forecast. They do strongly suggest where to look for initial condition errors that may have a big effect (in this case in the vicinity of the geopotential trough at midlevels). They also indicate what to expect from any (small) initial condition changes that may be applied.

When the mechanisms affecting the synoptic development are relatively simple, the adjoint fields have relatively simple interpretations (e.g., see Langland et al. 1995 or Rabier et al. 1992). Here, the processes of baroclinic instability and moist diabatic heating are acting simultaneously, and the adjoint fields are more difficult to interpret synoptically. They are best inter-

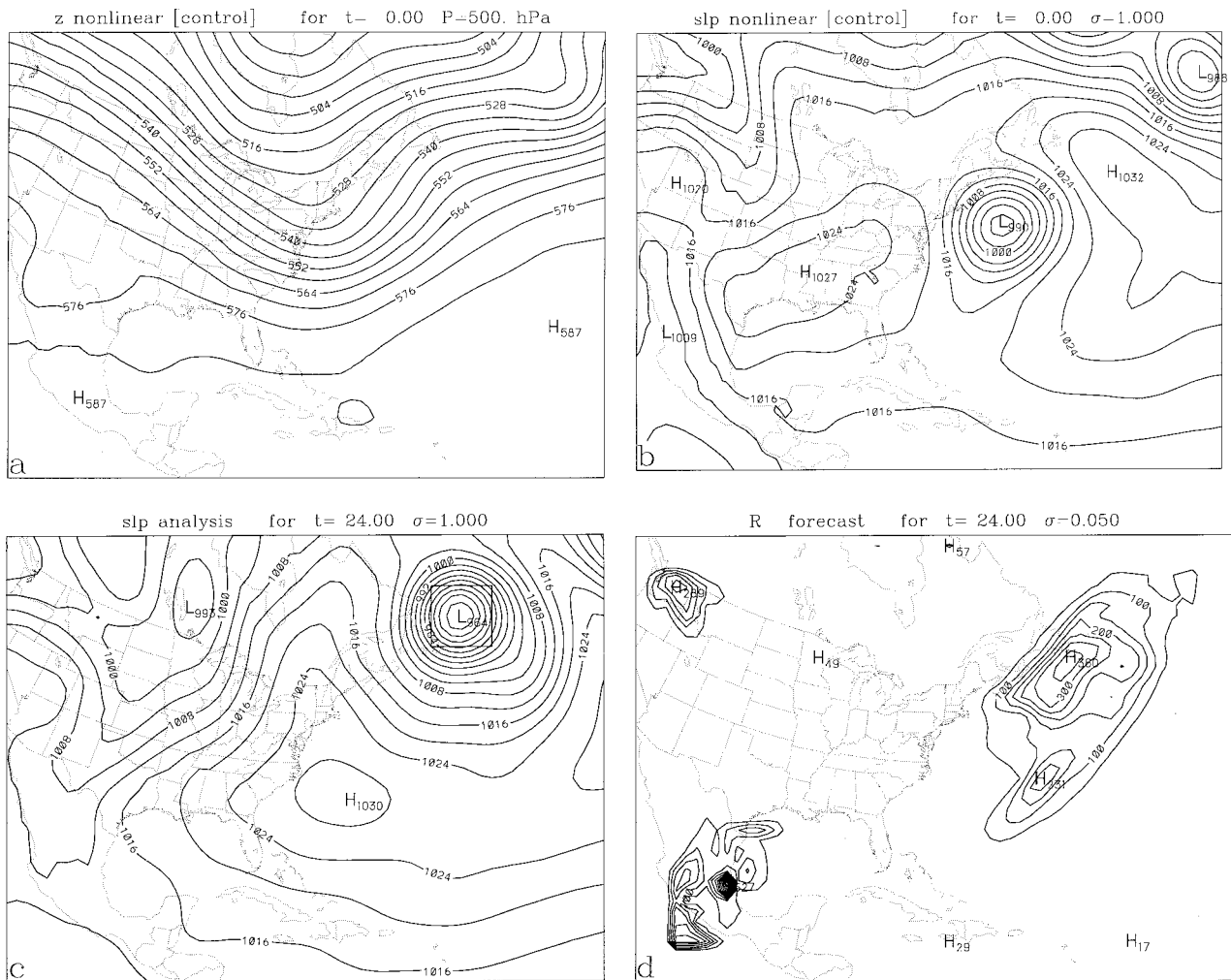


FIG. 1. The fields of (a) 50-kPa geopotential height at the initial time; fields of sea level pressure at the initial (b) and final (c) times; and (d) forecast precipitation accumulated during the 24-h forecast. Contour intervals are 60 m, 0.4 kPa, 0.4 kPa, and 0.5 cm, respectively. The square shown in (c) is the area over which the mean forecast vorticity is to be computed for the forecast aspect investigated.

preted by considering what a perturbation that has the same *structure* as the sensitivity field would cause. Such perturbations may be considered as “optimal” in the sense described in section 5.

Some adjoint results are likely anticipated. The sensitivity of J with respect to possible perturbations of the $\sigma = 0.65$ T field near Cape Hatteras, for example, may have been anticipated by considering the influence of possible changes of the sharpness of the initial 50-kPa geopotential trough on the forecast cyclone. Other implications of the adjoint results, however, may yield very new insights. Comparison of the magnitudes of the sensitivity fields in Figs. 2b–d, for example, indicates that a 1-K perturbation of T where the sensitivity has maximum magnitude has approximately the same effect as a $0.0006 \text{ kg kg}^{-1}$ perturbation of q where its sensitivity is a maximum but 9

times the effect of a 1 m s^{-1} perturbation of v where its sensitivity is a maximum. In this specific sense, therefore, J is much more sensitive to T and q than to v . Furthermore, the maximum sensitivity is located near 65 kPa, not at the tropopause or surface as one may guess by considering simple cyclone development arguments in terms of potential vorticity anomalies.

Note that none of these results would be as easily obtained by simply examining perturbed runs of the nonlinear model. Either too many runs would have to be made to obtain the same complete picture, or there is a strong chance that the impacts of simultaneously introduced perturbations would cancel (given that there are regions of both positive and negative sensitivity) yielding an incorrect impression of the possible impacts that can be obtained with other perturbations. If our interest is in knowing the impact on many J_i

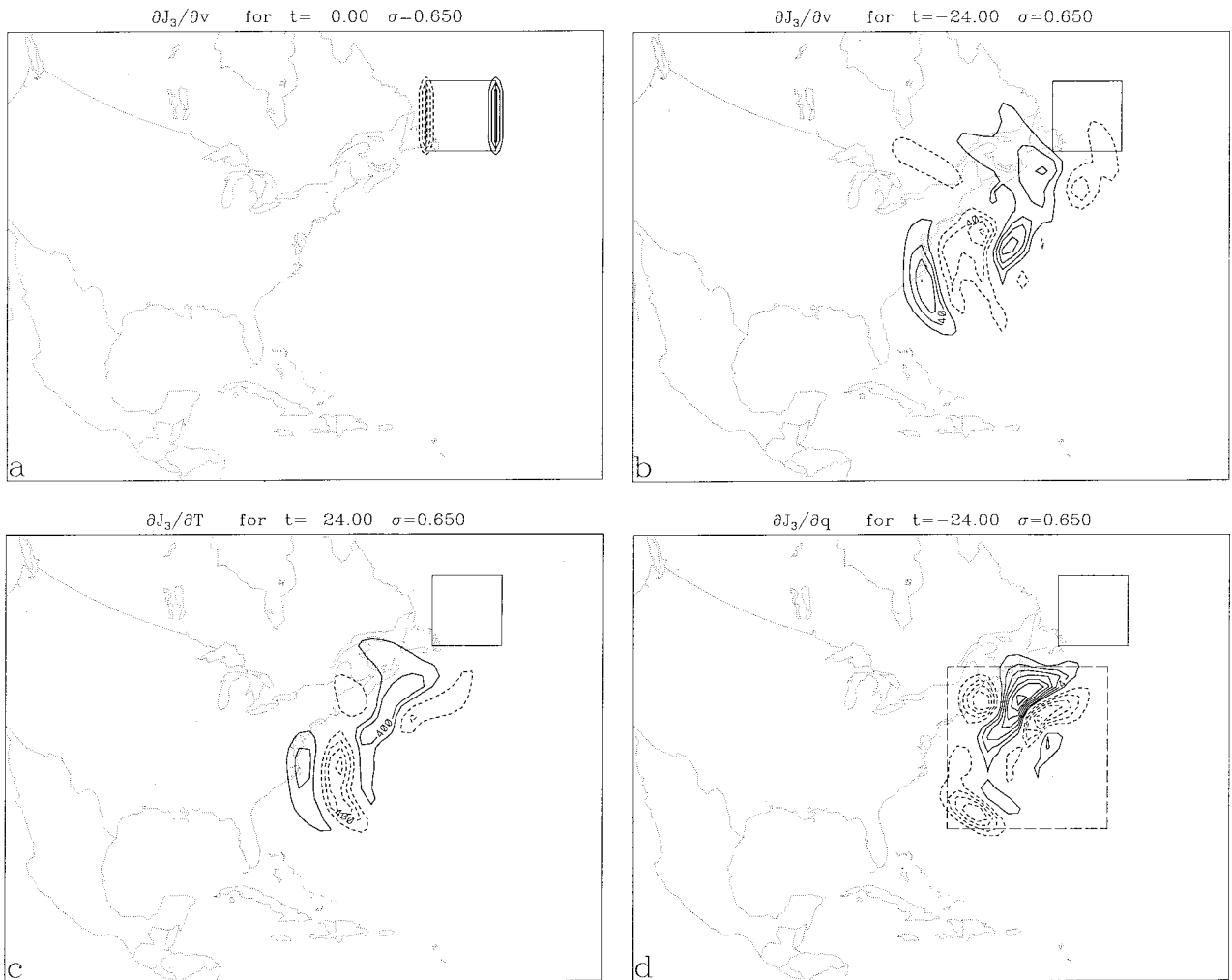


FIG. 2. The sensitivity of J (mean vorticity within the lower troposphere and area shown in Fig. 1c) with respect to (a) the field of v at the final (forecast verification) time, and (b) v , (c) T , and (d) q at the initial (analysis) time, all defined on the $\sigma = 0.65$ surface. Contour intervals are $1 \times 10^{-8} \text{ s}^{-1}(\text{m s}^{-1})^{-1}$, $2 \times 10^{-9} \text{ s}^{-1}(\text{m s}^{-1})^{-1}$, $2 \times 10^{-8} \text{ s}^{-1} \text{ K}^{-1}$, and $2 \times 10^{-5} \text{ s}^{-1}(\text{kg kg}^{-1})^{-1}$, respectively, negative contours are dashed, and 0-valued contours have been omitted for clarity. The square shown in solid lines is the area over which J is defined at the verification time. The dashed square indicates where q is perturbed at the initial time to test the accuracy of the adjoint results.

given a few perturbations, the nonlinear method would be appropriate, but a shift of a perturbation pattern by a few grid points may sometimes grossly change the results.

The adjoint can only produce the gradient for one J_n per application. Fortunately, often we are interested in only a few distinct J_n . Also, because it is based on a linearization, the sensitivity it suggests is only approximate. Interpretations must be made carefully and the accuracy of the corresponding tangent linear model should be examined for the cases and applications investigated. The computational cost of the adjoint of MAMS2 is about the same as an execution of the tangent linear or nonlinear models over the same time period.

As an indication of the accuracy of the adjoint result discussed here, the nonlinear model has been run with a perturbation of the initial condition within the $2000 \text{ km} \times 2000 \text{ km}$ area within the dashed lines shown in Fig. 2d. Only q in the bottom three model σ levels (approximately below 70 kPa) has been perturbed. At the locations and σ levels where $\partial J/\partial q$ is positive valued, the perturbation is 0.001 kg kg^{-1} ; where it is negative, the perturbation is $-0.001 \text{ kg kg}^{-1}$. If the perturbation is such as to make $q < 0$ at some location, the perturbation at that location is reduced in magnitude to make $q = 0$.

The control value of J is $8.39 \times 10^{-5} \text{ s}^{-1}$. The perturbation yields a $\Delta J = 1.04 \times 10^{-5} \text{ s}^{-1}$. If instead, the initial perturbations of q are multiplied by their corre-

sponding sensitivities and added according to (4), then the estimated change in J is $1.21 \times 10^{-5} \text{ s}^{-1}$. This is only a 17% error compared with the actual value obtained with the nonlinear model.

The effects on J due to other perturbations can be easily estimated using (4) without executing the nonlinear model again. For example, changing the signs of the previous perturbations should yield approximately the same magnitude change as earlier but with opposite sign. If the perturbation were the value 0.001 kg kg^{-1} (i.e., constant value) at the same points as earlier, the change of J is 7 times smaller, indicating that much cancellation occurs when summing over regions of positive and negative sensitivity. These two adjoint estimates were also checked with the nonlinear model, yielding errors less than 2% of the nonlinear changes.

These results are remarkably accurate, given the significant size of the perturbation and the fact that the primary way moisture perturbations affect the wind field is through highly nonlinear diabatic processes. Perturbations with different structures or magnitudes could yield very different accuracies, but our experience thus far suggests that these sensitivity fields have significant utility.

Note that the adjoint-determined result only applies to J being the mean vorticity in the verification box. These determined sensitivity fields do not, for example, indicate how the central pressure changes due to the same perturbations, although the two J and their sensitivities may be related (e.g., through geostrophy). Neither does it directly indicate “why” the estimated change occurs. Nevertheless, the sensitivity fields provide much useful information; for example, in the present example, it would likely have required a large ensemble of perturbed forecasts to obtain a significant change of J by avoiding cancellation between areas of oppositely signed sensitivity.

5. Adjoint applications

Sensitivity analysis has many applications. It may be used to examine model behavior, describing how input and output are related. It may be used to investigate model forecast errors, to highlight initial or boundary fields and locations that are more likely to be responsible for an error. Another use, yet to be exploited, is as a synoptic tool to determine what initial synoptic features are most strongly related to subsequent synoptic features (see, e.g., Langland et al. 1995).

Adjoint are indispensable for efficiently solving several types of optimization problems, which includes their most common applications to date. The simplest of these is to consider a linear (or linearized) J and ask what is the smallest perturbation of the model input that can produce a desired change ΔJ when the perturbation size is measured by some quadratic norm (i.e., sum of squares of perturbation components). Such information can be useful if we want to know if a discrepancy between forecast and analyzed values of J can be corrected by a reasonable modification to the forecast’s initial conditions.

As an example of this simple optimization problem, consider the simple norm that measures the sum of the squares of the perturbed input values:

$$I = \frac{1}{2} \sum_k w_k (\Delta a_k)^2, \quad (10)$$

where w is a weight that depends on the field type and maybe location. If the perturbation size is sufficiently small that the tangent linear approximation is acceptable, then both the perturbations of the model output and ΔJ are approximately linear functions of the perturbed input. The latter approximation is simply denoted by (4), and we can ask what minimizes (10) given the constraint (4). The result (e.g., determined using a Lagrange multiplier λ) is obtained by finding the Δa_k that minimize

$$K = \frac{1}{2} \sum_k w_k (\Delta a_k)^2 + \lambda \left(\Delta J - \sum_k \frac{\partial J}{\partial a_k} \Delta a_k \right), \quad (11)$$

where ΔJ is the prescribed desired change. The minimum of K occurs for the Δa_k that satisfy $\partial K / \partial a_k = 0$. The result is

$$\Delta a_k (\text{optimal}) = \frac{\lambda}{w_k} \frac{\partial J}{\partial a_k}, \quad (12)$$

which is just the gradient values multiplied by the indicated weights, with

$$\lambda = \Delta J \left[\sum_k \frac{1}{w_k} \left(\frac{\partial J}{\partial a_k} \right)^2 \right]^{-1} \quad (13)$$

so that the constraint (4) is satisfied.

Note that in this linearized example, one single application of the adjoint is sufficient to determine the optimal solution (i.e., no iteration is required). Furthermore, if the w depend only on field type and not location, then the *structures* of the adjoint-determined sensitivity fields are identical to those of the optimal perturbation field. In this specific sense, the sensitivity fields may therefore be considered as “optimal” structures. Similar results are obtained when the optimization problem is to determine the maximum ΔJ given a prescribed perturbation size I .

If J is not linear (nor linearized) or if the perturbation size is initially large or becomes large during the forecast such that the perturbation output is no longer approximately a linear function of the input, then iteration is required because $\partial J/\partial a_k$ is then an implicit function of $\mathbf{a} + \Delta \mathbf{a}$. Applications of this type are nicely discussed, for example, by Rabier et al. (1996) and Oortwijn and Barkmeijer (1995).

If J is a quadratic function of the perturbation itself, such as when we ask what will give us the largest size perturbation output [e.g., measured as by (10) except at some output time] given a constrained initial perturbation size $I = \text{constant}$, then the optimal solution is determined by an eigenvalue problem. Although there is usually a single, largest-growth solution, one can search for slower-growth solutions that are uncorrelated with the first (when measured using the same norm). These solutions have been called “optimal solutions” but now are usually called “singular vectors” for reasons best described in Ehrendorfer and Errico (1995).

The singular vectors may be interpreted as solutions to a generalized stability problem (Farrell and Ioannou 1996a,b). They can yield growing solutions (i.e., ones for which the norms, such as perturbation energy, grow with time) when no growing normal-mode solutions are found. This can occur when normal modes are nonorthogonal with respect to the norm; for example, when the sum of the values of the norm for individual normal modes is not equal to the norm of the sum of the modes. This is usually the case, except for simple, specifically designed problems. Unlike for normal-mode determination, the basic state whose stability is being examined need not be stationary (or quasi-stationary) in time for singular vectors to be determined. The singular vector analysis includes the normal-mode analysis as a special case, so it provides more general information.

The greatest attention to adjoints has been for their use to efficiently solve the computationally demand-

ing problem of four-dimensional variational data assimilation (4DVAR), which is schematically described in Fig. 3. Here, the goal is to produce the analysis that “best” fits observations, prior estimates of the fields to be analyzed (e.g., a “background” estimate produced by an earlier forecast valid at the analysis time), and our understanding of the physics that relates observations of different types and times to the fields to be analyzed. The latter implies use of a model that may be used as either a strong (Lewis and Derber 1985; Talagrand and Courtier 1987) or weak (Derber 1989; M. Zupanski 1993) constraint. The measure of how well the analysis fits all this information should include weights consistent with the statistics of errors associated with each piece of information (Tarantola 1987; Daley 1991). The fit may also include measures designed to constrain noise, such as due to inertia-gravity waves (e.g., Courtier and Talagrand 1990).

Figure 3 indicates the following. Point B is a background estimate of the atmospheric state at time t_1 produced by an earlier forecast, with indicated error bars. Point O_1 is an observation of the atmospheric state at approximately the same time, with indicated error bars. Point A is a likely value for the analysis, given by the intersection of the information available at t_1 . It produces a forecast, F, for time t_2 . This disagrees with the observation O_2 valid at that time. An adjoint model is applied to a measure of the differences $F - O_2$ and $B - O_1$ (for all fields and observations) to make a new analysis A^* also consistent with the information at t_1 . It produces a significantly different forecast F^* due to the modeled atmospheric instabilities that is also consistent with O_2 . The expected result is that, even at times $t > t_2$, the forecast started at A^* remains better than the one started at A and also better than one started at an A_2 produced by an intermittent data assimilation scheme. There are more optimal ways of using data over the period $t_1 \leq t \leq t_2$ or $t \leq t_2$, and A^* will only be statistically better than A if all the information has been used properly, with proper accounting for all the corresponding error statistics.

The 4DVAR fitting function defines a J as a function of the analysis, with parameters determined by the input information and their error statistics. The adjoint is used to determine the local gradient of J with respect to the analysis fields, which is then applied to some algorithm to find the analysis that yields the best fit (i.e., minimum J). Although such an optimization problem was posed in meteorology by Sasaki (1969), it has awaited the advent of adjoint models to become

computationally practical. When designed properly, with good estimates of the error statistics, good gravity wave control, and a good model, 4DVAR should be better able to assimilate data by better connecting information in time than previous methods have done.

As with previous methods, such as optimal interpolation (Daley 1991), 4DVAR uses past observations, as they have affected the background estimates, in addition to present ones. Unlike previous methods, however, it also uses future observations, in the sense that if we wait 6–24 h beyond the time for which the analysis is to be valid (plus the time required to obtain the data), the later observations can be used in conjunction with a forecast model to help constrain the analysis. For example, knowing the time evolution of moisture patterns we can infer winds, and seeing developments in unstable regions we can better specify precursor patterns. Since even single observations used in this way can impact many fields over a significant area, the analysis produced may even be better than one produced using the old methods at the later time [see Thépaut et al. (1993) and Thépaut et al. (1996) for some examples and further references].

Note that without careful attention to all the many aspects of the data assimilation problem, use of an adjoint model does not by itself imply that better analyses will be produced. In particular, using the model as a strong constraint in 4DVAR will result in adjustments of the analysis to compensate for any significant model errors so the resulting forecast can still come close to the observations. Also, the results will be sensitive to precisely how the fitting function is defined, and therefore any poor assumptions about the statistics of forecast and observational errors will likely degrade the accuracy of the analysis (e.g., see Fillion and Errico 1997).

The 4DVAR problem is computationally demanding, even with an adjoint to make minimizing J more efficient. Unlike many other proposed methods, however, it may be feasible in an operational environment [e.g., compare the computational demands for 4DVAR described by Courtier et al. (1994) with those for the method described by Bennett et al. (1996)].

Adjoint models can also be used for efficient determination of model parameters, for example, for those appearing in the model's parameterization schemes. This is similar to the problem of data assimilation, except that instead or in addition to tuning model initial conditions, the best fit of forecasts with respect to the model parameters is determined. There are some significant differences between the two prob-

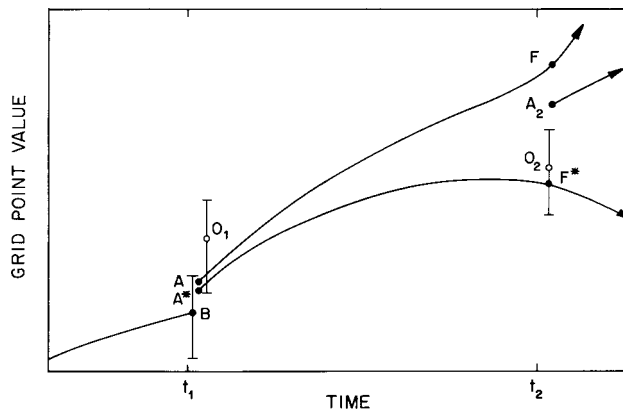


FIG. 3. Schematic of four-dimensional variational data assimilation.

lems, however, when the specification of parameters should be robust (i.e., apply well to all cases, not just those for which the fitting has been performed), physically reasonable (requiring the consideration of constraints in the form of inequalities), and simultaneously satisfy several criteria of acceptability.

The newest application of adjoints is for assisting the “targeting” of observations. The motivation here is to use sensitivity fields of some kind to determine where it is most important to produce an accurate initial condition for a forecast. Where the sensitivity is large, any significant error in the initial conditions there will have a significant impact on the forecast J and therefore on the accuracy of its prediction. Similar errors where the sensitivity is low will have little affect on the forecast J . It is therefore critical to keep the initial errors small in the sensitive regions. This can be done by, for example, deploying aircraft to make observations in those places. The locations will depend on how the “importance” is measured (i.e., on the J_{η} used). They will also depend on the accuracy of the nonlinear model used to generate the forecast as well as the accuracy of its adjoint used to determine the sensitivity (see, e.g., Palmer et al. 1997; Langland et al. 1996).

Where the sensitivity is greatest is not necessarily the location that should be targeted. The expected size of the analysis error at the location must also be considered. If the analysis there is expected to be very accurate, it is not necessary to make more observations there, regardless of the sensitivity. Also, having more observations where they are important does not imply the subsequent analysis and forecast will be better. Especially if they are in an area of strong sensitivity, even small observational errors or marginally

misspecified error correlation functions can produce unacceptable forecast errors. Targeting will likely produce better forecasts only if the data assimilation system used is sufficiently good and its estimation of error statistics sufficiently accurate.

6. Adjoint limitations

The greatest limitation to the application of adjoints is that the results are useful only when the linearized approximation is valid. The tangent linear or adjoint results may be correct in that they accurately describe the first-order Taylor series approximation to the behavior of perturbations in our application; that is, the behavior as the perturbation size becomes infinitesimally small. Those results may be useless, however, if our real interest is in the behavior of some finite-sized perturbation, as it almost always is. In particular, if J or the model is nonlinear, there will likely be a perturbation size for which the linearization becomes inadequate in the sense that both (1) using a tangent linear model and (4) using an adjoint suggest the wrong response to the perturbation in the nonlinear model.

The perturbation size may become large because it is prescribed so initially, or it may become large because the perturbation size grows with time, for example, as when a dynamic instability exists. For the latter reason, there is generally a time at which the behavior of almost any perturbation enters the nonlinear regime in most nonlinear atmospheric models [i.e., the effects of chaos occur as described by Lorenz (1969); see also Tribbia and Baumhefner (1988)]. Adjoint applications are therefore usually limited to certain short time spans. How short will depend on the size of initial perturbations considered, the types of physics to be considered (e.g., dry dynamics versus moist convection) and the structure of the perturbation (does the perturbation grow or decay during the period considered and what physics primarily acts upon it). It is therefore difficult to specify a general time limit for adjoint applications, but experience with numerical weather prediction models and initial perturbations that resemble expected initial-condition errors suggests that if only dry physics is considered, a linearization may remain valid for up to 3 days for synoptic-scale features. When the moist physics associated with precipitation is significant, this time-scale may be greatly reduced (e.g., see Park and Droegemeier 1995), although good results have been

obtained at synoptic scales for periods as long as 1 day (ER).

Some physical parameterization schemes used in models are formulated with conditionals: depending on the state of the solution at any considered time, the functions that determine the result of the physics can be different. One example is the often-used simple nonconvective precipitation scheme that produces a nonzero effect only when a modeled air parcel is supersaturated. Such formulations can be formally nondifferentiable, although in a temporally and spatially discrete formulation, almost all model solutions will fall on one side or the other of such conditions at each time and thus are differentiable along the discrete model trajectory as required for existence of the model's Jacobians. Rather than impairing the formulation of the tangent linear and adjoint model versions, the effect of the conditionals is therefore to reduce the usefulness of the linear approximations made. A perturbation in the nonlinear model may change the sense of a conditional, causing effects that the linearization does not describe. This can be amended by considering all the possible trajectories but would be highly impractical when the number of degrees of freedom is very high, as in models used for weather prediction. Alternatively, the conditionals can be removed by replacing them with some smooth functions. Ideally this should be done without compromising the modeling of the concerned physics. It can even be argued that any conditionals are unrealistic since they likely do not account for smoothing effects due to the uncertainty associated with the statistical nature of the parameterization scheme. These questions have been investigated in part (Xu 1996; ER; Verlinde and Cotton 1993; Zou et al. 1993; D. Zupanski 1993) and their investigation will undoubtedly continue.

Sometimes the forecast aspects that interest us are associated with nondifferentiable J . For example, in a gridpoint model we may be interested in determining the point at which a local pressure minimum is obtained for defining the location of a cyclone's center. The algorithm to determine this point involves comparing pairs of numbers and choosing the minimum. Such an algorithm is nondifferentiable. It may be that, for this example, an alternative algorithm that determines an equivalent result but that is differentiable may be developed, but there are likely aspects of interest for which such alternatives are impossible. Also, the accuracy of the first-order Taylor series approximation will vary with the forecast measures used as well as with the cases to which they are applied.

Therefore, great care should be taken when choosing a forecast aspect to be measured as well as when interpreting the result.

Many adjoint applications have been misinterpreted in the past. An adjoint result (i.e., pattern of sensitivity) does not necessarily indicate what locations or fields are most important. Since it does indicate where sensitivity is greatest, however, it provides an invaluable piece of information required to determine what is most important. Neither do optimally derived perturbations necessarily show where errors in forecast initial conditions are, although again, they should offer invaluable insight. Lastly, using an adjoint in a data assimilation scheme does not necessarily mean more accurate analyses are obtained. That accuracy depends on details of many aspects of the assimilation scheme. In this application, the adjoint is simply a very useful tool, but not a guarantor of success.

7. The future of adjoints

Derivation of tangent linear equations and adjoint equations for models as complicated as those used for numerical weather prediction is usually straightforward, although tedious. If the software for the nonlinear model is designed well, the software for the corresponding tangent linear and adjoint models is most easily produced by a line by line analysis of the nonlinear model software [e.g., directly from its FORTRAN code, treating each subroutine or line as one of the functions B_n appearing in (8)]. Simple rules exist for this purpose (e.g., see Talagrand 1991; Giering and Kaminski 1996). In fact, computer software exists that can produce C or FORTRAN adjoint models from similarly coded nonlinear models (e.g., Giering and Kaminski 1997; Rostaing et al. 1993; Bischoff 1994), although, under some conditions, these automatic adjoint generators may produce adjoint codes that are incorrect or computationally too inefficient.

Testing of the tangent linear and adjoint software is also straightforward and rigorous if all that is required is that it be properly derived from the parent, nonlinear model. The development and testing can be quite tedious, however, especially since the testing methods can be quite sensitive to even what may be considered very minor errors; that is, software errors usually become apparent unlike when nonlinear forecasting models are developed and the “truth” is known imprecisely. Errors originally in the nonlinear model

may simply be transcribed to the tangent linear and adjoint versions, but since the development and testing usually requires detailed reexamination of the nonlinear model, errors in the nonlinear model are often found too. Some undesirable aspects of the nonlinear model solution that were considered tolerable in its former applications (such as very small amplitude numerical noise) may become intolerable as more is demanded of the model solutions; for example, when the small difference between two (control and perturbed) nonlinear model solutions is examined, the signal to noise ratio may be dramatically reduced, rendering the noise intolerable. One often unforeseen result of developing an adjoint version should therefore be reexamination and subsequent improvement of the nonlinear model itself.

Developments in the field of adjoint applications in meteorology have been fast paced. There has sometimes not been time for robust and detailed analysis, for example, involving many synoptic cases and types of diagnostics. Sometimes important aspects of the problem are neglected, such as gravity wave control in 4DVAR studies. Some statements or results are misleading or erroneous. In particular, extreme care must be taken when attempting to generalize any reported results. In the earliest papers on adjoint applications, the mathematical presentation was often formidable and unnecessary in the discrete model framework almost always employed. For all these reasons, readers may find some existing papers confusing, incomplete, or unreadable. A fairly complete and partially annotated bibliography of most papers on adjoint applications and data assimilation published prior to 1993 appears in Courtier et al. (1993). I especially recommend many of the papers coauthored by either P. Courtier or F. Rabier for their readability and accuracy. Many novices in the field have found Errico and Vukićević (1992) useful, although their adjoint had many approximations and much simpler presentations can now be made. Several papers describing both general and particular applications of adjoints in data assimilation may be found in Ghil et al. (1997).

Often in meteorology we can only indirectly answer the questions that interest us. In particular, prior to the development of adjoint models, we had to infer sensitivity from impact studies as described in section 2. As adjoint models become more available and as their applications are better understood by the community, they should make a very large impact on how we do science and how we understand the atmosphere.

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