Numerical Weather Prediction

A comparison of two methods of deriving the tangent linear model

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Abstract

The tangent linear model has become widely used within numerical meteorology, both as an explicit model of perturbation growth and as a means of determining the adjoint model. In this study we look at two ways of finding such a linear model; the usual method of linearizing a discrete nonlinear model is compared with the method used at the UK Meteorological Office, in which a numerical scheme is applied to the continuous linearized equations. The methods are compared using a simple initial value problem. The two methods produce different linear models, which may exhibit quite different behaviour if model instabilities are present. We demonstrate problems which may arise when applying the standard test of a tangent linear model.

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1 Introduction

Recent years have seen an increase in the development of adjoint models within numerical weather prediction. Their efficiency in providing the gradient of an objective function makes them particularly useful for solving large optimization problems. Their applications in weather forecasting include 4-dimensional variational assimilation (4D-Var) [12], and the calculation of singular vectors to determine sensitive regions within a meteorological field. The latter are useful within a variety of problems, for example the study of forecast error, the determination of initial perturbations for ensemble forecasts and the targetting of atmospheric observations [5], [7].

In determining the adjoint model, use is made of the linearization of the nonlinear model around a background trajectory, the tangent linear model. In certain applications, such as the incremental formulation of 4D-Var, the tangent linear model itself is also used explicitly to model the evolution of a small perturbation [3]. The calculations made with such models require that the tangent linear model represents the nonlinear evolution of a perturbation to a good approximation. The satisfaction of this requirement will, in general, depend on the particular meteorological situation.

In order that the tangent linear model correctly represents the first order part of the nonlinear model, it is usually obtained by a linearization of the discrete form of the nonlinear model. This can be done directly from the nonlinear model source code, a process known as *automatic differentiation*. The adjoint model is then obtained by transposing the source code of the linear model [2], [6]. This method has come to be widely accepted as the way that tangent linear and adjoint models should be developed.

However, there are some inherent difficulties with this approach. Recent work by Polavarapu et al. [9] has shown that errors may occur when the interpolation procedures of semi-Lagrangian schemes are linearized in this manner. A problem arises if the perturbed departure point is in a different grid interval from the original departure point. In this case, for infinitesimal variations, the tangent linear model will correctly represent the first order term of the nonlinear model if and only if the interpolating function has a continuous first derivative. For finite perturbations it was found that this condition is also necessary, but it is no longer sufficient.

Polavarapu and Tanguay [8] have also looked at the practical problems of determining the linear model in this way when iterative processes are involved, for example in semi-Lagrangian schemes or elliptic solvers. For such schemes the linearization of the discrete scheme requires information of the background trajectory to be stored for each iteration. In schemes which perform several iterations of a solution procedure on each time step, this leads to very large storage requirements. Other work in this area has studied the difficulties of treating the linearization of discontinuous processes within physical parametrizations (for example [1]).

At the UK Meteorological Office an alternative approach to developing the linear model has been taken. Beginning with the continuous nonlinear equations, we first linearize to form a set of continuous linear equations. These linear equations are then discretized to form the linear model, following as closely as possible the integration scheme used in the nonlinear model. The adjoint model is derived from the discrete linear model.

There are two main advantages to this approach. The first is based on the premise that what we want to model is the true evolution of a perturbation in the atmosphere. The model can therefore be based more on physical principles and can make some small approximations to the true tangent linear model. If the magnitude of such approximations is no greater than that of the linearization error, then this should not affect the accuracy of the calculations, but will allow significant savings to be made to the running costs of the models.

The second advantage to this approach is that it is possible to avoid some of the problems with the particular kinds of schemes discussed above. For example, the numerical model we are working with requires the solution of a 3-dimensional Helmholtz equation, which is performed using an iterative solver (see [4] for full details of the scheme). Our approach to forming the linear model allows us to apply the same solver to solve a Helmholtz equation within the linear model and avoids the need to linearize the iterative procedure.

Sirkes and Tziperman [11] have previously shown differences between forming the adjoint model from the continuous linearized equations and forming it from the discrete nonlinear model. However they do not examine the linear model itself, which plays an important role in incremental 4D-Var. In this study we concentrate on the properties of the linear model. We look at the two approaches to forming the model, either discretizing the nonlinear equations and then linearizing, or linearizing the nonlinear equations and then discretizing the continuous linear equations thus formed. The effects of possible further approximations are not considered. We study the problem for the case of an ordinary differential equation (ODE) initial value problem, first using a general linear multistep method and then a particular nonlinear method. For this study the examples chosen are fairly simple, and there is no guarantee that the results presented here will extend directly to a system of partial differential equations present in numerical weather prediction models. However, even these simple examples highlight some general points which we will need to look at when we turn our attention to the full system.

In Section 2 we set up the problem we wish to model. In Sections 3 and 4 we then present an analysis of the different methods of linearization, using a general linear multistep scheme and a particular Runge-Kutta scheme. The results of the analysis for the Runge-Kutta scheme are illustrated with some numerical results in Section 5. We then make a short comment on the linearization state in Section 6, before presenting our conclusions in Section 7.

2 The problem

We consider the general ODE initial value problem for a function $x(t)$ of the form

$$\frac{dx}{dt} = f(x), \;\; t \in [a,b], \; x(a) = x_0, \tag{1}$$

where f is explicitly a function in x only. The linearization of this equation is

$$\frac{d(\delta x)}{dt} = f'(x)\delta x, \tag{2}$$

where

$$f'(x) \equiv \left.\frac{df}{dx}\right|_{x,t}.$$

Equation (2) is the *tangent linear equation* of (1). We note that since $x = x(t)$, the coefficient of δx in (2) varies with time. This must be taken into account when applying schemes that require coefficients from different time levels. The procedure we follow is to apply a numerical scheme to equation (1) and then linearize this scheme. The results from this are compared to those obtained by applying the original numerical scheme directly to equation (2).

Before doing this, it is desirable to say something about the existence of solutions to these equations. We assume that equation (1) has a unique solution. This is true if f is continuous on some interval $[x_a, x_b]$ and satisfies a Lipschitz condition

$$\| \, f(x_1) - f(x_2) \, \| \leq L \;\; \| \, x_1 - x_2 \, \|$$

for all $x_1, x_2 \in [x_a, x_b]$. L is the Lipschitz constant.

In order to show that the tangent linear problem (2) has a Lipschitz condition and therefore a unique solution, we first note that for given perturbations $\delta x_1, \delta x_2$ to a state $x(t)$, we have

$$\| f'(x)\delta x_1 - f'(x)\delta x_2 \| \leq \| f'(x) \| \| \delta x_1 - \delta x_2 \| .$$

Hence, if $f'(x)$ is bounded in $[x_a, x_b]$, we can choose

$$L = \max\{\| f'(x) \| : x \in [x_a, x_b]\}$$

to give the required condition. A bound on $f'(x)$ is therefore a sufficient condition for a solution to exist and so this is assumed in our analysis.

Given that both equations can be solved, we can now look at the problem of producing the discrete tangent linear model. First we clarify the notation used in the remainder of this paper. Given a model variable $x = x(t)$, the value of the analytic solution at time t_i is written $x(t_i)$. The model solution at this time, which will be an approximation to the true value, we denote x_i.

3 Linear multistep methods

If we consider a general k-step linear method applied to equation (1), we have

$$\alpha_k x_{n+k} + \alpha_{k-1} x_{n+k-1} + \ldots + \alpha_0 x_n = \Delta t[\beta_k f_{n+k} + \beta_{k-1} f_{n+k-1} + \ldots + \beta_0 f_n], \quad (3)$$

where $f_i \equiv f(x_i)$.

A linearization of this scheme produces

$$\begin{aligned} \alpha_k \delta x_{n+k} &+ \alpha_{k-1}\delta x_{n+k-1} + \ldots + \alpha_0 \delta x_n \\ &= \Delta t[\beta_k f'_{n+k}\delta x_{n+k} + \beta_{k-1} f'_{n+k-1}\delta x_{n+k-1} + \ldots + \beta_0 f'_n \delta x_n]. \end{aligned} \quad (4)$$

This is exactly the same as the result of applying the full scheme (3) to the tangent linear equation (2). Hence, for the case of a linear multistep method, linearizing the discrete model is the same as discretizing the linear equation.

4 Nonlinear methods

The conclusion of the previous section does not hold when we apply a nonlinear numerical method to the problem. To illustrate this, we use the example of a two-stage Runge-Kutta scheme for solving

$$\frac{dx}{dt} = g(x,t),$$

given by

$$
\begin{aligned}
k_1 &= \Delta t\, g(x_i, t_i), \\
k_2 &= \Delta t\, g(x_i + \Delta t\, g(x_i, t_i), t_i + \Delta t), \\
x_{i+1} &= x_i + \frac{1}{2}(k_1 + k_2).
\end{aligned} \tag{5}
$$

Applying this scheme to the nonlinear equation (1), we note that the function f does not depend explicitly on t and therefore we have

$$
\begin{aligned}
k_1 &= \Delta t\, f(x_i), \\
k_2 &= \Delta t\, f(x_i + \Delta t\, f(x_i)),
\end{aligned} \tag{6}
$$

which gives the model solution

$$
x_{i+1} = x_i + \frac{\Delta t}{2} \left\{ f(x_i) + f(x_i + \Delta t\, f(x_i)) \right\}. \tag{7}
$$

Linearizing this scheme gives

$$
\begin{aligned}
\delta x_{i+1} &= \delta x_i + \frac{\Delta t}{2} \{ f'(x_i) \delta x_i \\
&+ f'(x_i + \Delta t\, f(x_i))[1 + \Delta t\, f'(x_i)] \delta x_i \}.
\end{aligned} \tag{8}
$$

However, if we apply the nonlinear scheme (5) to the tangent linear equation (2), noting the time dependence of the coefficient of δx, we obtain

$$
\begin{aligned}
\delta x_{i+1} &= \delta x_i + \frac{\Delta t}{2} \{ f'(x_i) \delta x_i \\
&+ f'(x_{i+1})[1 + \Delta t\, f'(x_i)] \delta x_i \}.
\end{aligned} \tag{9}
$$

A comparison of (8) and (9) shows that they are very similar, but with x_{i+1} in the second equation being replaced by an estimate of this in the first. In the second scheme, however, x_{i+1} is given by the more accurate estimate obtained from (7), which implies that

$$
\begin{aligned}
\delta x_{i+1} &= \delta x_i + \frac{\Delta t}{2} \{ f'(x_i) \delta x_i \\
&+ f'(x_i + \frac{\Delta t}{2} \left\{ f(x_i) + f(x_i + \Delta t\, f(x_i)) \right\})[1 + \Delta t\, f'(x_i)] \delta x_i \}.
\end{aligned} \tag{10}
$$

It is clear that equations (8) and (10) are not the same for a general function f. Hence with a nonlinear scheme, it does matter whether we linearize or discretize first. We therefore wish to examine the two linear models (8) and (10) to see if we can say something about the errors in each of them. The error can be analysed in two ways; a comparison of the linear and nonlinear evolutions of a perturbation determines the validity of the models under given conditions, whereas an analysis of the truncation error shows the order of accuarcy of the models. We treat each of these in turn.

4.1 Comparison of perturbations

The usual way of testing the validity of a tangent linear model is to see how well it models the behaviour of a perturbation in the nonlinear model ([10]). The method can be summarized as follows:

Let M_i be a given nonlinear model which maps a model state at time t_i to one at time t_{i+1}, and let $x_i = M(x_0, t_i)$ represent the model state vector after being integrated from time t_0 to time t_i, starting from an initial state x_0. Then given an initial state of the model x_0 and a small perturbation δx_0, we can run the model twice starting from the two different conditions x_0 and $x_0 + \delta x_0$. The difference between these two runs at any particular time is the perturbation, N, evolved in the nonlinear model, given by

$$N = M(x_0 + \delta x_0, t_i) - M(x_0, t_i). \tag{11}$$

Now define M_i' to be the Jacobian matrix of the model operator with respect to its state vector at time t_i and $M'(x_0, t_i)$ the repeated application of this operator from time t_0 to time t_i around the trajectory given by $M(x_0, t_i)$, i.e.

$$M'(x_0, t_i) = \prod_{j=0}^{i-1} M_j'. \tag{12}$$

Then $M'(x_0, t_i)$ is the solution operator of the tangent linear model. By a Taylor series expansion we find that

$$M(x_0 + \delta x_0, t_i) - M(x_0, t_i) = M'(x_0, t_i)\delta x(t_0) + O(\delta x^2). \tag{13}$$

Thus, to first order, the solution operator of the tangent linear model applied to $\delta x(t_0)$ is equal to the perturbation N calculated from the runs of the nonlinear model. A comparison of these two quantities therefore allows us to determine the validity of the linear model.

Since this test is based on a linearization of the model, it favours the linear model produced by linearizing the discrete scheme, which for this problem is the exact tangent linear model according to the definition (12). We can show this by looking at the perturbed nonlinear equation

$$\frac{d}{dt}(x + \delta x) = f(x + \delta x). \tag{14}$$

Applying the Runge-Kutta scheme and subtracting the solution of the unperturbed equation (7), we obtain to first order in δx equation (8), the linearization of the discrete scheme. Hence the use of this error measure to determine the validity of a linear model must contain the caveat that it only determines to what extent the linear part of the discrete nonlinear model is captured. It does not provide a comparison with the evolution of a perturbation according to the continuous equations. The effect of this will be seen more clearly when we look at some numerical results in Section 5.

4.2 Truncation error

It is useful to calculate the truncation errors in both the linear schemes, to check the accuracy to which they solve the linear equation. In order to do this we would like to compare with the truncation error of the scheme applied to the nonlinear equation, and so this is calculated first.

Let us denote the truncation error of the nonlinear model as τ_{NL}. Then by the definition of truncation error and using (7), we have

$$\tau_{NL} = \frac{x(t_{i+1}) - x(t_i)}{\Delta t} - \frac{1}{2}\left\{f(x(t_i)) + f(x(t_i) + \Delta t\, f(x(t_i))\right\}.$$

Noting that $x(t_{i+1}) = x(t_i + \Delta t)$, we can expand this around time t_i and also expand the second function about $f(x(t_i))$. Using the fact that

$$\begin{aligned}
\frac{dx}{dt} &= f(x(t)),\\
\frac{d^2x}{dt^2} &= f(x(t))f'(x(t)),\\
\frac{d^3x}{dt^3} &= [f'(x(t))]^2 f(x(t)) + f''(x(t))[f(x(t))]^2,
\end{aligned}$$

we find

$$\begin{aligned}
\tau_{NL} &= \left(\frac{1}{6}f(x(t_i))[f'(x(t_i))]^2 - \frac{1}{12}f''(x(t_i))[f(x(t_i))]^2\right)\Delta t^2\\
&+ O(\Delta t^3). \qquad (15)
\end{aligned}$$

By this we see that the scheme is second order in time.

Now we wish to examine the truncation errors for the two linear schemes (8) and (10), which we denote τ_1 and τ_2 respectively. First we must be clear about what these quantities mean. For the discretization (10) of the linear equation (2), the truncation error is defined in the usual way with respect to the true solution of the equation that the scheme approximating. However, when we look at the linearization of the nonlinear discrete system (8), we do not have a clear definition of truncation error, since this scheme is not designed as an approximation to any particular equation. For comparison therefore, we take the truncation error with respect to the solution of the same linear equation (2).

For the linearization of the discrete scheme (8), the truncation error is found to be

$$\begin{aligned}\tau_1 &= \frac{\delta x(t_{i+1}) - \delta x(t_i)}{\Delta t} - \frac{1}{2}\{f'(x(t_i))\delta x(t_i) \\ &+ f'(\,x(t_i) + \Delta t f(x(t_i))\,)[1 + \Delta t f'(x(t_i))]\delta x(t_i)\}. \qquad (16)\end{aligned}$$

Now expanding $\delta x(t_{i+1}) = \delta x(t_i + \Delta t)$ around t_i and expanding the last term of the equation around $f'(x(t_i))$, and using

$$\begin{aligned}\frac{d(\delta x)}{dt} &= f'(x(t))\delta x + O(\delta x^2), \\ \frac{d^2(\delta x)}{dt^2} &= f''(x(t))f(x(t))\delta x + [f'(x(t))]^2\delta x + O(\delta x^2), \\ \frac{d^3(\delta x)}{dt^3} &= f'''(x(t))[f(x(t))]^2\delta x + 4f''(x(t))f'(x(t))f(x(t))\delta x \\ &+ [f'(x(t))]^3\delta x + O(\delta x^2),\end{aligned}$$

we find that to order δx

$$\begin{aligned}\tau_1 &= \Big(\frac{1}{6}[f'(x(t_i))]^3 + \frac{1}{6}f''(x(t_i))f'(x(t_i))f(x(t_i)) \\ &- \frac{1}{12}f'''(x(t_i))[f(x(t_i))]^2\Big)\delta x(t_i)\Delta t^2 + O(\delta x(t_i)\Delta t^3). \qquad (17)\end{aligned}$$

We note first of all that this is second order. A simple manipulation shows that it is equal to the linearization of (15).

Turning now to what happens when we discretize the continuous linear equation, we find that the truncation error is

$$\begin{aligned}\tau_2 &= \frac{\delta x(t_{i+1}) - \delta x(t_i)}{\Delta t} - \frac{1}{2}\{f'(x(t_i))\delta x(t_i) \\ &+ f'(x(t_i) + \frac{\Delta t}{2}\{f(x(t_i)) + f(x(t_i) + \Delta t\, f(x(t_i)))\})[1 + \Delta t f'(x(t_i))]\delta x(t_i)\}, \qquad (18)\end{aligned}$$

and with the same cancellations as in the previous case, this reduces to

$$\begin{aligned}\tau_2 &= \Big(\frac{1}{6}[f'(x(t_i))]^3 - \frac{1}{12}f''(x(t_i))f'(x(t_i))f(x(t_i)) \\ &- \frac{1}{12}f'''(x(t_i))[f(x(t_i))]^2\Big)\delta x(t_i)\Delta t^2 + O(\delta x(t_i)\Delta t^3). \qquad (19)\end{aligned}$$

Again we see that this is second order, but this time it is not the linearization of the truncation error of the nonlinear scheme.

For both linear schemes the second order accuracy in time is only second order with respect to the linear equation (order δx). There are terms in τ_1 and τ_2 of order δx^2 and higher which are only first order in time, but these vanish in the linear approximation.

5 Example

To illustrate the theory let us consider the simple example $f(x) = x^2$, i.e.

$$\frac{dx}{dt} = x^2, \tag{20}$$

with $t \in [0, 10]$ and $x(0) = x_0$. The analytic solution to this equation is given by

$$x = \frac{x_0}{1 - x_0 t}. \tag{21}$$

By considering a perturbation δx to the problem (20), we obtain the equation for the exact nonlinear evolution of a perturbation,

$$\delta x(t) = \frac{\delta x_0}{(1 - (x_0 + \delta x_0)t)(1 - x_0 t)}. \tag{22}$$

Applying the Runge-Kutta scheme (5) to (20), we obtain the discrete nonlinear model

$$x_{i+1} = x_i + x_i^2 \Delta t + x_i^3 \Delta t^2 + \frac{x_i^4 \Delta t^3}{2}, \tag{23}$$

which is second order in time, with truncation error

$$\tau_{NL} = \frac{x(t_i)^4 \Delta t^2}{2} + \sum_{n=4}^{\infty} x(t_i)^{n+1} \Delta t^{n-1}. \tag{24}$$

The linearization of the analytic equation (20) is

$$\frac{d(\delta x)}{dt} = 2x\delta x, \tag{25}$$

which has the solution

$$\delta x(t) = \frac{\delta x_0}{(1 - x_0 t)^2}. \tag{26}$$

To find the linear model by the first method, we linearize the discrete scheme (23) to obtain

$$\delta x_{i+1} = (1 + 2x_i \Delta t + 3x_i^2 \Delta t^2 + 2x_i^3 \Delta t^3)\delta x_i, \tag{27}$$

The second linear model is determined by applying the discrete scheme (5) to the linear equation (25). This gives

$$\delta x_{i+1} = \delta x_i + x_i \Delta t \delta x_i + x_{i+1} \Delta t[1 + 2x_i \Delta t]\delta x_i. \tag{28}$$

Then, using the estimate of x_{i+1} from (23), we have

$$\begin{aligned} \delta x_{i+1} &= \delta x_i + x_i \Delta t \delta x_i + \Big(x_i + x_i^2 \Delta t + x_i^3 \Delta t^2 \\ &\quad + \frac{x_i^4 \Delta t^3}{2}\Big) \Delta t[1 + 2x_i \Delta t]\delta x_i \\ &= (1 + 2x_i \Delta t + 3x_i^2 \Delta t^2 + 3x_i^3 \Delta t^3 + \frac{5}{2} x_i^4 \Delta t^4 + x_i^5 \Delta t^5)\delta x_i. \end{aligned} \tag{29}$$

Substituting the correct solution into both these schemes, and using equations (20) and (25) and their derivatives, we find the following truncation errors:

- for the linearization of the discrete scheme to order δx

$$\begin{aligned}\tau_1 &= 2x(t_i)^3\Delta t^2\delta x(t_i) + 5x(t_i)^4\Delta t^3\delta x(t_i) + 6x(t_i)^5\Delta t^4\delta x(t_i) \\ &+ \sum_{n=6}^{\infty}(n+1)x(t_i)^n\Delta t^{n-1}\delta x(t_i), \qquad (30)\end{aligned}$$

which we note is the linearization of (24);

- for the discretization of the linear equation

$$\begin{aligned}\tau_2 &= x(t_i)^3\Delta t^2\delta x(t_i) + \frac{5}{2}x(t_i)^4\Delta t^3\delta x(t_i) + 5x(t_i)^5\Delta t^4\delta x(t_i) \\ &+ \sum_{n=6}^{\infty}(n+1)x(t_i)^n\Delta t^{n-1}\delta x(t_i), \qquad (31)\end{aligned}$$

which can be seen is different from τ_1, with a smaller principal term.

5.1 Numerical experiments

In order to compare the linear and nonlinear evolution of the perturbations, some numerical experiments were performed with this example, according to the method described in Section 4.1. The schemes were coded and the nonlinear model was run from two slightly different initial conditions x_0 and $x_0 + \delta x_0$ at time $t = 0$. The difference between these two runs was then compared with each of the linear models initialized with the perturbation δx_0 at $t = 0$. The first experiment used values of $x_0 = -2.5$ and $\delta x_0 = -0.1$ and a time step $\Delta t = 0.25$. The output is shown in Figure 1. The solid line shows the difference between the two nonlinear runs, the dashed line shows the scheme formed by linearizing the discrete scheme (27) and the dotted line shows the discretization of the linear equation (29). Also plotted with diamonds is the true nonlinear variation of a perturbation calculated from the analytic expression (22). For this experiment the solid line and the dashed line are almost identical. We see that both linear models approximate well the true nonlinear variation.

The experiment was then repeated with larger time steps, first for $\Delta t = 0.35$ and then for $\Delta t = 0.5$. The output from the first of these is shown in Figure 2. The solution trajectory from the model formed by discretizing the linear equation moves away from the other curves. This model thus seems to be less accurate in representing both the true nonlinear variation and the evolution in the discrete nonlinear model, despite having a smaller truncation error.

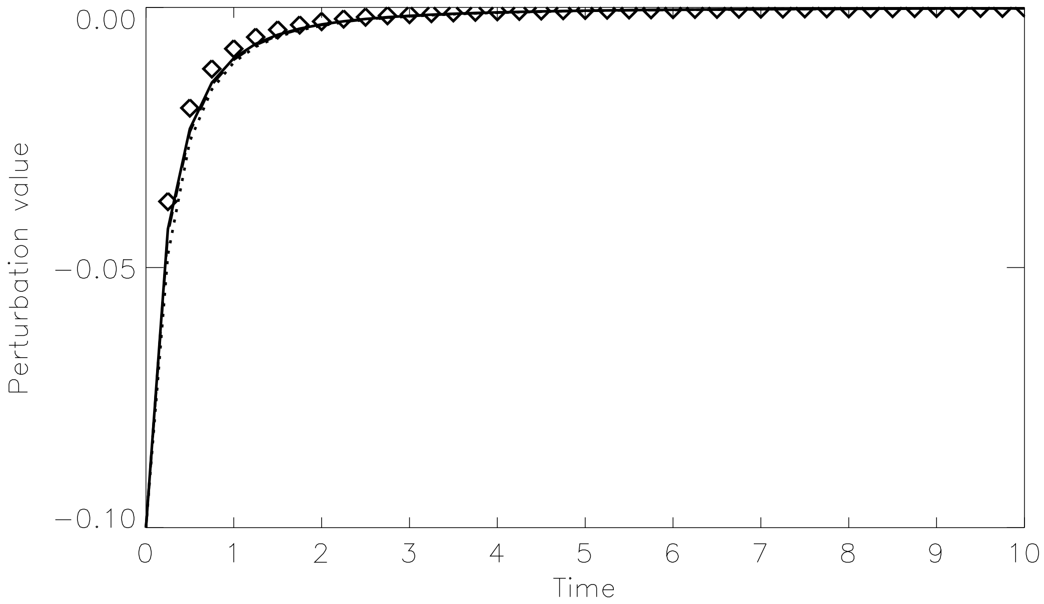

Figure 1: Plot of perturbation against time for $\Delta t = 0.25$. The solid line indicates the evolution in the nonlinear model, the dashed line shows the linearization of the discrete scheme, the dotted line shows the discretization of the linear equation and the diamonds indicate the true nonlinear variation.

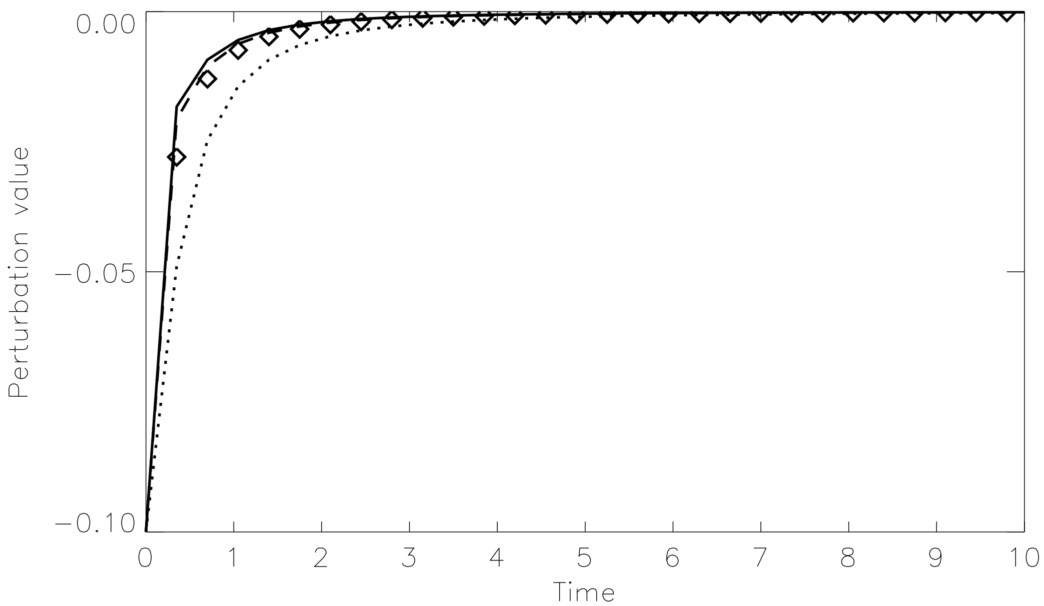

Figure 2: As Figure 1, with $\Delta t = 0.35$.

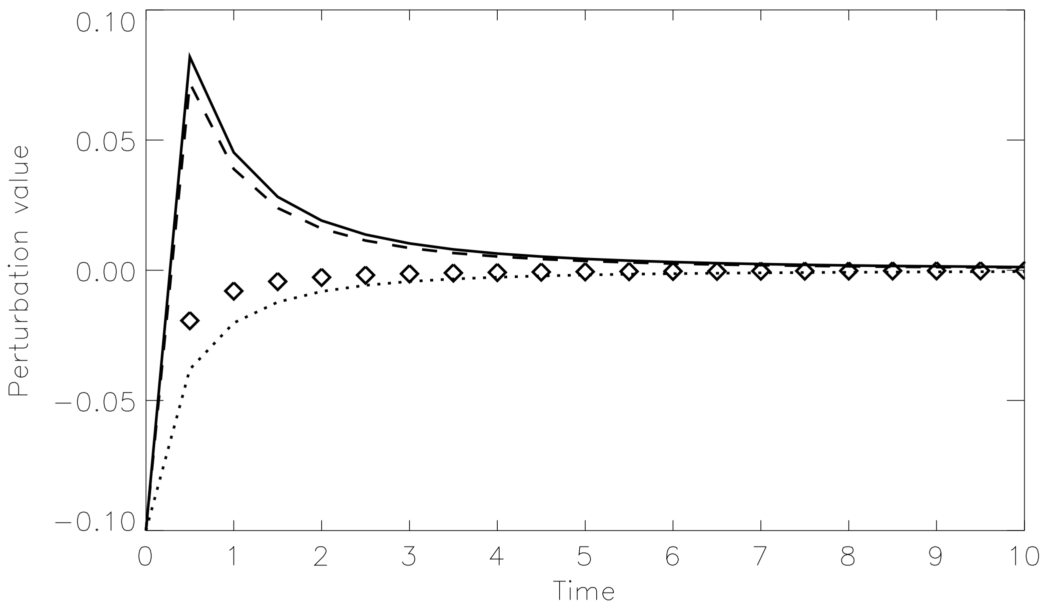

Figure 3: Plot of perturbation against time for $\Delta t = 0.5$. The solid line indicates the evolution in the nonlinear model, the dashed line shows the linearization of the discrete scheme, the dotted line shows the discretization of the linear equation and the diamonds indicate the true nonlinear variation.

However, when the time step is increased even further, to a value of 0.5, a different behaviour is seen. The output from this experiment is shown in Figure 3. In this case the difference between the two runs of the discrete nonlinear model is quite different from the true nonlinear evolution of the perturbation. The linearization of the discrete scheme follows closely the difference between the two discrete nonlinear runs, whereas the discretization of the linear equation is closer to the true nonlinear variation.

To explain the peak in these results which makes the two linear schemes so different, it is useful to look at the behaviour of the numerical solution of the nonlinear equation. The solution from the runs of the nonlinear model is shown in Figure 4. The dotted line indicates the model run with $\Delta t = 0.25$, the dashed line with $\Delta t = 0.5$ and the solid line is the analytic solution. The global error of these runs is shown in Figure 5. It can be seen that doubling the time step gives a large increase in the error of the model solution, showing that the scheme itself is inaccurate with the larger time step. The effect of this inaccuracy on the difference between the perturbed and unperturbed runs is that the perturbation can change sign. This can be seen in Figure 3; the solid line shows the initial negative perturbation becoming positive during the nonlinear model run, whereas

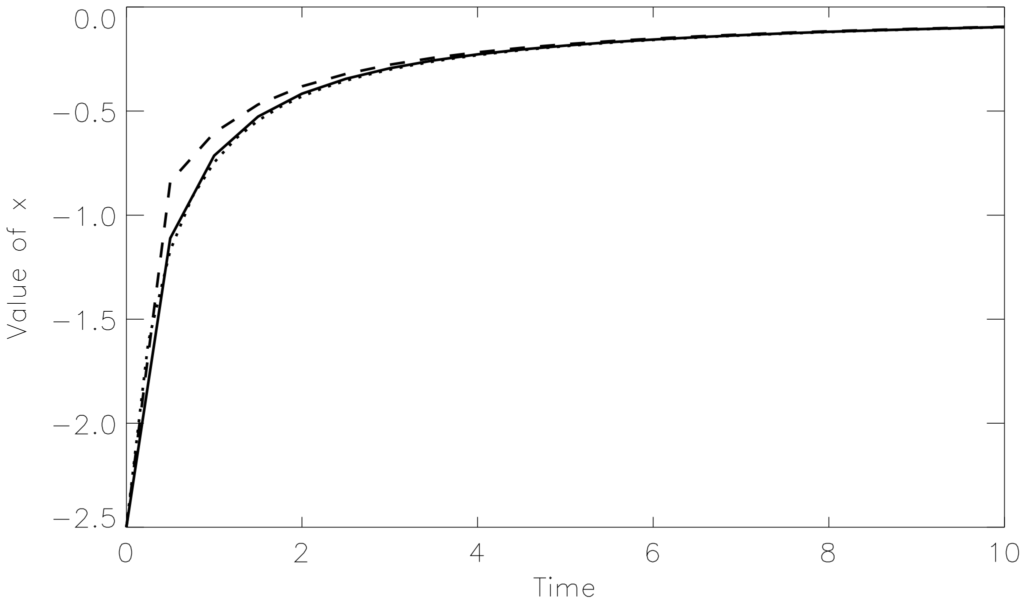

Figure 4: Solution of nonlinear model runs. The dotted line is for $\Delta t = 0.25$ and the dashed line is for $\Delta t = 0.5$. The solid line indicates the analytic solution of the nonlinear problem.

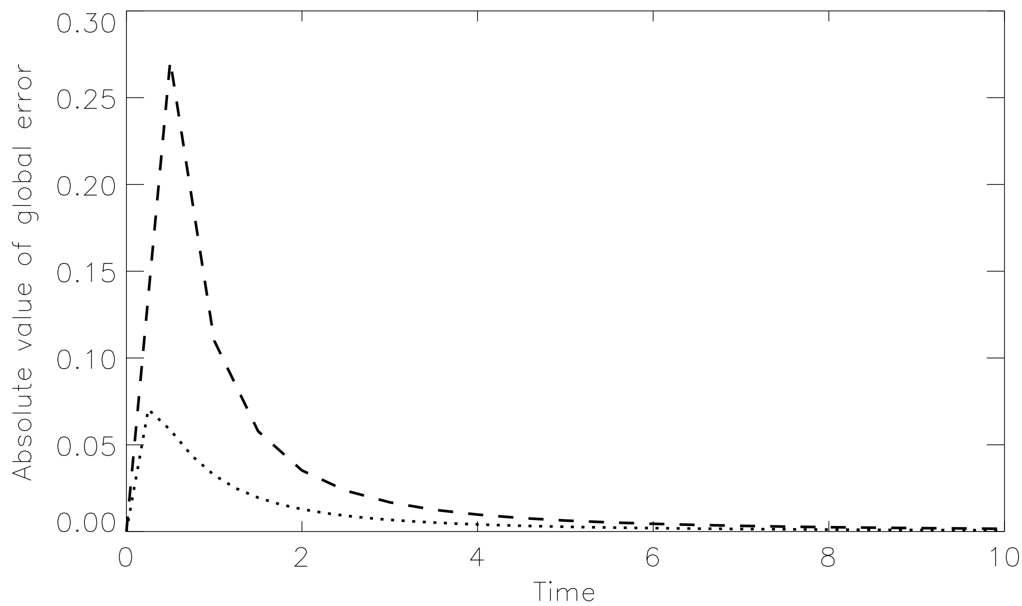

Figure 5: Global error of nonlinear model runs. The dotted line is for $\Delta t = 0.25$ and the dashed line is for $\Delta t = 0.5$.

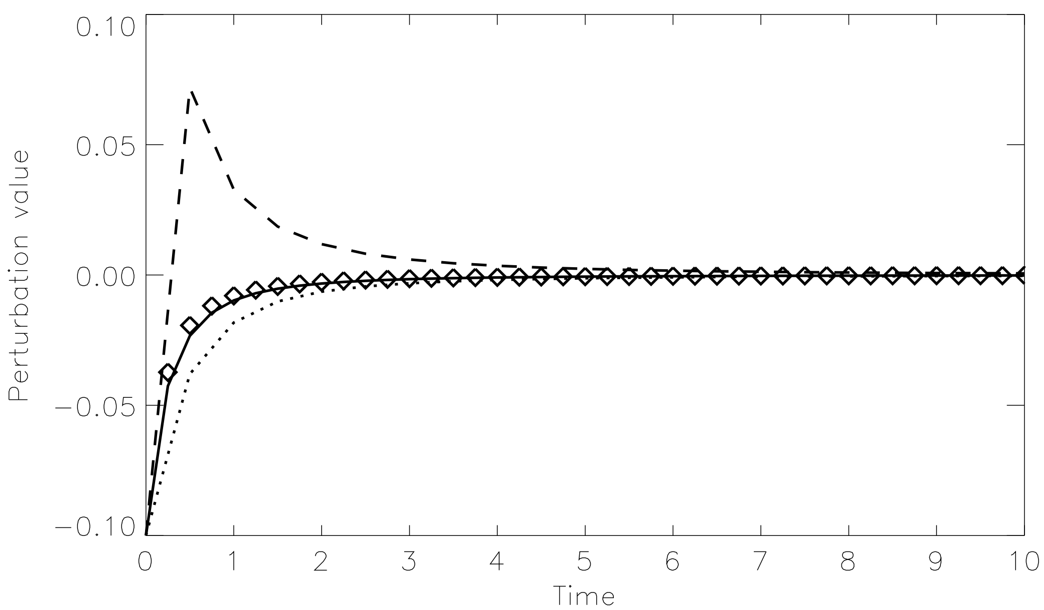

Figure 6: As Figure 3, but with the nonlinear model run with $\Delta t = 0.25$ and the linear models run with $\Delta t = 0.5$.

the true nonlinear variation, shown by the diamonds, remains always negative.

If we consider the true nonlinear variation (22), then for given initial values x_0 and δx_0 both less than zero, we see that $\delta x(t)$ cannot change sign. If we examine the analytic solution to the linear equation (26), we see also that δx at any time t is always a positive factor times the initial δx and thus cannot change sign. Hence the analytic solutions to both the nonlinear and linear problems tell us that an initial negative perturbation must remain negative throughout the model run. Thus the behaviour of the perturbation in the discrete nonlinear model is one which is not allowed by the analytic solution.

Turning now to the linear models, we wish to understand why the solution of that formed by linearizing the discrete scheme (the dashed line in Figure 3) follows the erroneous nonlinear model solution. In particular, we wish to determine whether this is an effect of an incorrect linearization state or a feature of the scheme itself. The experiments were therefore repeated, using a time step of $\Delta t = 0.25$ in the nonlinear model run, and then using the linearization state from this to force the linear models with a time step of $\Delta t = 0.5$. The result of this is shown in Figure 6. From this experiment we see that a more correct linearization state is not enough to prevent the perturbation from changing sign in the linear model formed from the linearization of the discrete scheme. The linear model is unstable even though the nonlinear model is well-behaved. The problem must therefore be inherent in the scheme of the linear model. We therefore analyse further the linear schemes, to understand how their behaviour changes with time step.

5.2 Analysis of numerical results

We first consider the stability of the schemes. Applying the Runge-Kutta scheme (5) to the ODE

$$\frac{dy}{dt} = \mu y,$$

where μ is a negative constant, gives the linear stability limit

$$\Delta t < -\frac{2}{\mu}.$$

Hence with $\mu = 2x$, as in our linear equation, we find that for stability we require

$$\Delta t < -\frac{1}{x}. \tag{32}$$

For $x = -2.5$ this gives a time step limit of $\Delta t < 0.4$.

This limit also holds for the linear model formed by linearizing the discrete nonlinear scheme. If we define the *amplification factor* λ_i of the linear scheme as

$$\lambda_i = \frac{\delta x_{i+1}}{\delta x_i},$$

then for an initial negative perturbation to remain negative we require that λ_i is always positive. A simple analysis of (27) shows that (32) is a necessary and sufficient condition for this.

To illustrate this we plot λ_i for the scheme, for a range of values of x and Δt. This is shown in Figure 7. We see that for $x = -2.5$ the amplification factor becomes negative for time steps Δt greater than 0.4, as predicted by the analysis.

In contrast, the scheme formed by discretizing the linear equation allows a larger time step for any particular value of x than that given by the above analysis. In this case, the scheme allows for the variation of μ in time, thus making it more stable for larger time steps than the model formed by linearizing the discrete nonlinear scheme. This can be seen in the plot of its amplification factor in Figure 8. A comparison with Figure 7 shows a greater range of values for which λ_i remains positive. In particular, for $x = -2.5$ and time step $\Delta t = 0.5$, λ_i is positive with value 0.38.

In order to compare the accuracy of the linear schemes, we define the *local* error of each scheme at time t_{i+1} by

$$E = \delta x(t_{i+1}) - \delta x_{i+1},$$

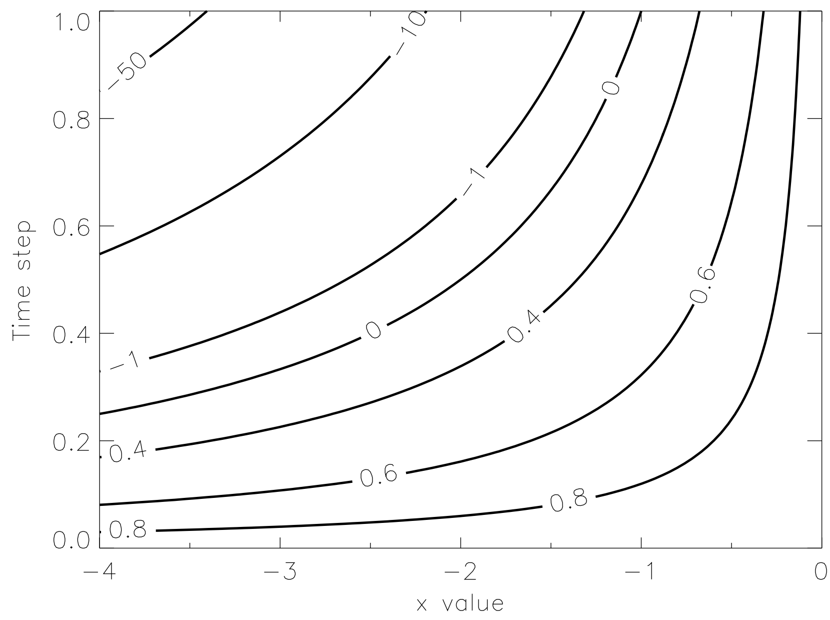

Figure 7: Amplification factor for various time steps and values of x: Linearization of discrete scheme.

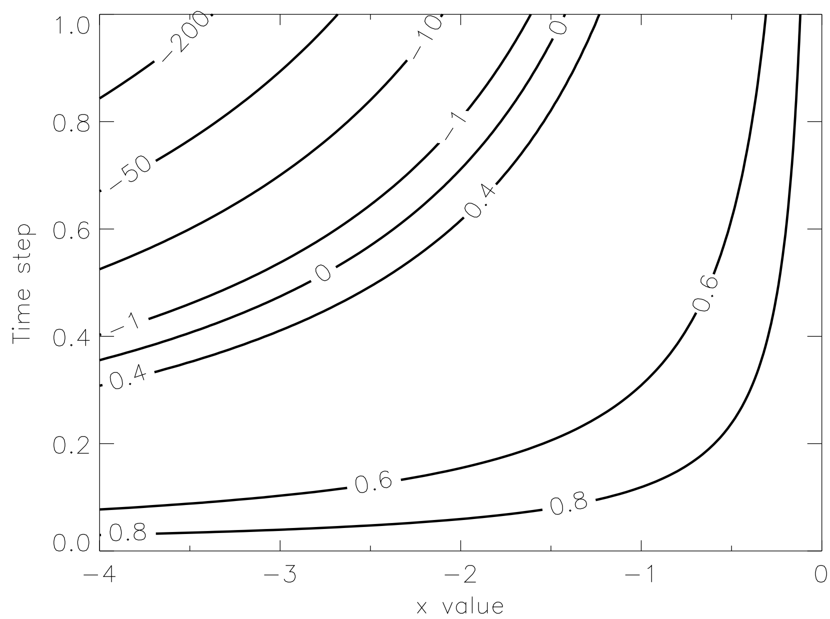

Figure 8: Amplification factor for various time steps and values of x: Discretization of linear equation.

where we assume $\delta x_i = \delta x(t_i)$ and $x_i = x(t_i)$. Then, expanding about time t_i we find the following local errors after one time step:

- for the linearization of the discrete scheme to order δx

$$E_1 = [2x(t_i)^3\Delta t^3 + 5x(t_i)^4\Delta t^4 + 6x(t_i)^5\Delta t^5 + O(x(t_i)^6\Delta t^6)]\delta x(t_i); \tag{33}$$

- for the discretization of the linear equation

$$E_2 = [x(t_i)^3\Delta t^3 + \frac{5}{2}x(t_i)^4\Delta t^4 + 5x(t_i)^5\Delta t^5 + O(x(t_i)^6\Delta t^6)]\delta x(t_i). \tag{34}$$

The higher order terms of these errors are identical, and so we can write an exact expression for their difference,

$$E_1 - E_2 = [x(t_i)^3\Delta t^3 + \frac{5}{2}x(t_i)^4\Delta t^4 + x(t_i)^5\Delta t^5]\delta x(t_i). \tag{35}$$

A simple analysis shows that within the limits of stability, the magnitude of the error E_2 is greater than that of E_1 wherever

$$-1 < x\Delta t < -\frac{1}{2}.$$

For a value of $x = -2.5$ this corresponds to a time step range of $0.2 < \Delta t < 0.4$, and so explains the relative accuracy of the two linear solutions when $\Delta t = 0.35$. When the time step is less than 0.2, we find that the scheme formed by the discretization of the continuous linear equation is more accurate.

6 Linearization state

Within each of the linear models we find a dependence on $x(t)$, the state about which the model has been linearized. This state is called the linearization state. From equation (9) we note that the discretization of the linear equation depends on $f'(x(t))$ at times t_i and t_{i+1}, where $t_{i+1} = t_i + \Delta t$. In operational use we may want to replace both of these with some average value of the linearization state, since storing the values at every time step may be too costly. There are different ways that this can be done. One way is just to use the value of the linearization state at time t_i everywhere. However, calculation of the truncation error for this scheme shows it to be first order in time; that is, the accuracy of the original scheme is reduced.

Since a reduction in accuracy is undesirable, the next natural thing to try is to find an average state in the middle of the time step, which we will write x_m. This gives the scheme

$$\begin{aligned} \delta x_{i+1} &= \delta x_i + \frac{\Delta t}{2}\{f'(x_m)\delta x_i \\ &+ f'(x_m)[1+\Delta t f'(x_m)]\delta x_i\}. \end{aligned} \tag{36}$$

Note that this is not just the same scheme (5) with values at the intermediate time level, since this formula would imply that $k_1 = f'(x_m)\delta x_i$, which contains variables at two different time levels. Applying this scheme to the general linear equation, the truncation error τ_3 is

$$\begin{aligned} \tau_3 &= \frac{\delta x(t_{i+1}) - \delta x(t_i)}{\Delta t} - \frac{1}{2}\Big[2f'(x(t_m))\delta x(t_i) \\ &+ \Delta t[f'(x(t_m))]^2 \delta x(t_i)\Big]. \end{aligned} \tag{37}$$

We have looked at two different ways of calculating the intermediate value. We can either take the average of the values of x at the ends of the time step, *i.e.*

$$x_m = \frac{1}{2}\Big(x_i + x_{i+1}\Big), \tag{38}$$

or we could take the value of the model state at the middle of the time step

$$x_m = x_{i+\frac{1}{2}}. \tag{39}$$

This second option requires the nonlinear model, which generates the linearization state, to be run at a higher time resolution than the linear model in order to produce the intermediate values. An expansion of the truncation error finds that both of these options are second order accurate.

Although it may be argued that this is not a fair comparison, since by changing the time of the linearization state we are changing the numerical scheme, this is in fact what we do in practice. In the perturbation forecast model of the Meteorological Office we apply the scheme of the nonlinear model to the linear equations, and afterwards decide where to take our linearization state. Hence it is important to know to what extent the choice of linearization state can affect the accuracy of the model.

To illustrate the effects of the choice of linearization state, the numerical experiment of the previous section was repeated twice, using the scheme given by (36) and a time step of 0.5. For the first run x_m was taken to be equal to x_i, and in the second run the value of x_m defined by (38) was used. The results are shown by the asterisks in Figures 9 and 10 respectively. It is seen that using the value at the start of the time step, giving only a first order approximation, does indeed degrade the results. The evolution is no

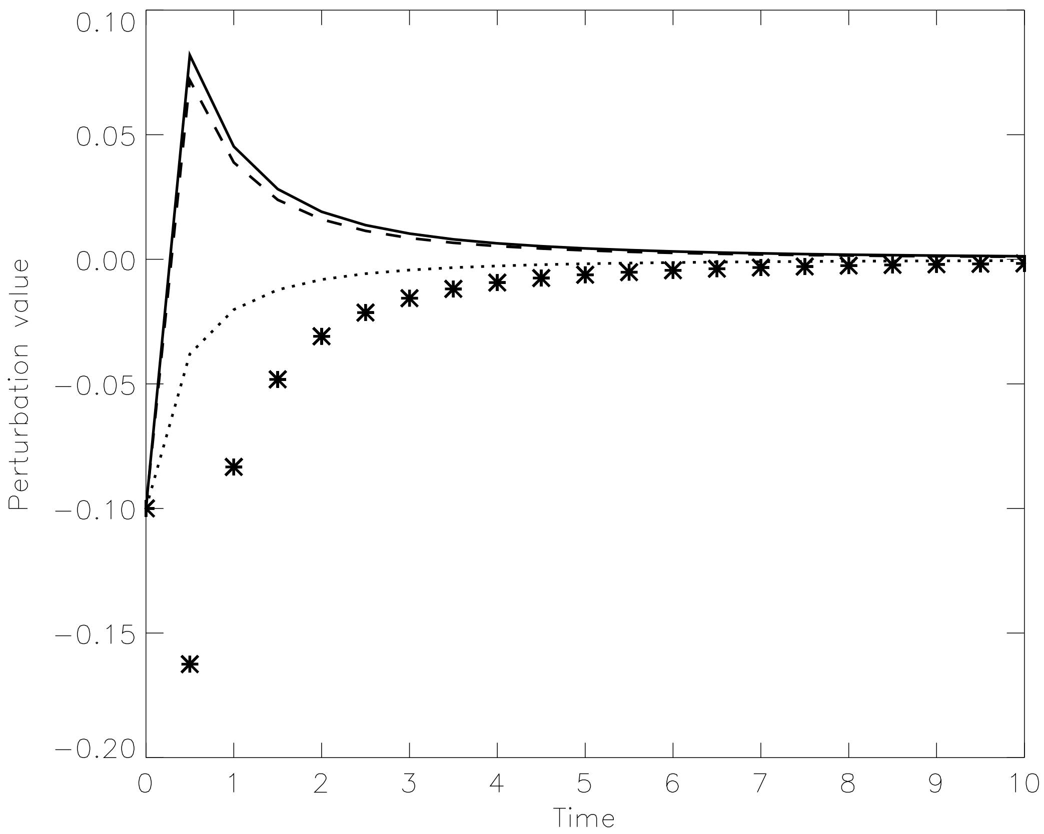

Figure 9: As Figure 3, with the asterisks showing the evolution when the linearization state is taken at the start of the time step.

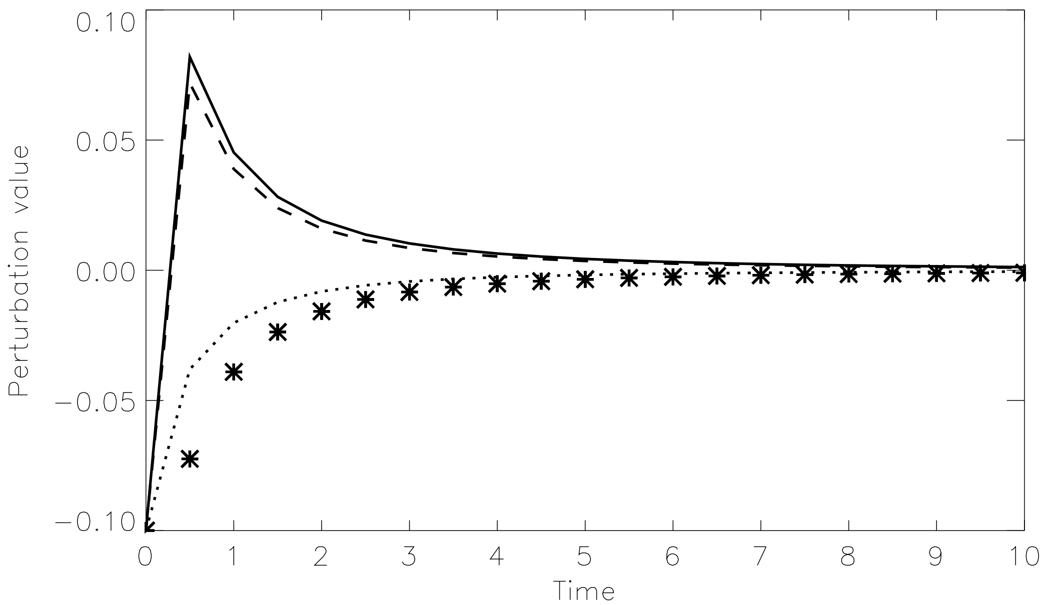

Figure 10: As Figure 3, with the asterisks showing the evolution when the linearization state is taken at the midpoint of the time step.

longer monotonic, but has an undershoot in the early stages of the run. Averaging the linearization state to the midpoint of the time step instead results in a much closer solution to the true discretization of the linear equation.

7 Conclusions

Although this study has looked at only a very simple example of a numerical scheme, it has demonstrated some details which must be taken into account when coding a tangent linear model or an approximation to it. It is clear that the two methods of deriving the tangent linear model lead to different results; applying a nonlinear numerical scheme to the continuous tangent linear equation is not the same as linearizing the discrete nonlinear model. The linear models thus formed may have different stability characteristics and so may exhibit different behaviours in some circumstances. Sirkes and Tziperman [11] found similar properties when looking at different ways of determining the adjoint model; the model formed by taking the adjoint of the finite difference scheme could contain computational modes not present when taking the discretization of the continuous adjoint. Our study indicates that such differences may also occur when forming the tangent linear model.

These differences may become particularly important if we wish to run the linear model at a lower temporal resolution than the nonlinear model. In practice this will be the case in 4D-Var, since many iterations of the linear model will be required and means to reduce the cost of the linear model must therefore be sought. Our numerical results illustrate that it is possible that the linear model formed by linearizing the discrete scheme may become unstable for time steps at which the other linear model remains stable. There may of course be situations in which the contrary holds. However, an advantage we see in applying the discrete scheme to the continuous linear equation is that the stability characteristics may be more easily controlled by careful choice of the scheme.

A corollary of these results is that the testing of a linear model must be performed with a good understanding of the nature of the numerical scheme. The usual method of testing such a model by comparing its output to the evolution of a perturbation in a nonlinear model will indicate how well the linear model represents the behaviour of the discrete nonlinear model. This is expected from the theoretical analysis and has been illustrated with numerical experiments. However, if the limitations of the numerical scheme are not understood, the linear model will not necessarily indicate the true evolution of a perturbation in reality, for example a perturbation to the atmosphere, and so may not be valid for applications which require this. It is therefore necessary to keep in mind the particular application for which the model is required.

For the example considered in this study, we have also shown that both methods of linearization produce models of the same order of accuracy. However, the relative magnitudes of the local error for each model may be dependent on the time step being used. If we apply a slightly modified version of the scheme to the continuous linear equation, for example by using the linearization state at a different time level, then the order of accuracy may be reduced. In practice we may want to do this, approximating the true linearization state by one valid at a different time, in order to reduce storage costs. Further investigation will be required to see the effect on accuracy this will have for the schemes actually used at the UK Meteorological Office.

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