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LETTERS TO THE EDITOR

Comments on "Tangent linear and adjoint of 'on–off' processes and their feasibility for use in 4-dimensional variational data assimilation"

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1. Introduction

The recent paper of Zou (*Tellus* 1997, henceforth refereed to as Z97) examines tangent linear and adjoint of "on–off" processes and their feasibility for use in 4-dimensional variational data assimilation. Some of the formulations presented in the analytical study (Section 4) of Z97 appear to be similar to the original results of Xu (1996a, henceforth referred to as X96a), but there are substantial discrepancies in the derivations of the adjoint and in the understandings of the problems between X96a and Z97. The main issues are as follows.

2. Should on–off switches cause discontinuities in the gradient? What kind of generalization is really needed?

It was stated at the end of Subsection 3.2 in Z97 that, "since the gradient of J is discontinuous at switching points, a more general definition of the derivative of the costfunction is required to understand the result of adjoint model integration". This statement and related statements in the last paragraph of Subsection 3.3 have the following problems.

(a) First, on–off switches in the solution do not

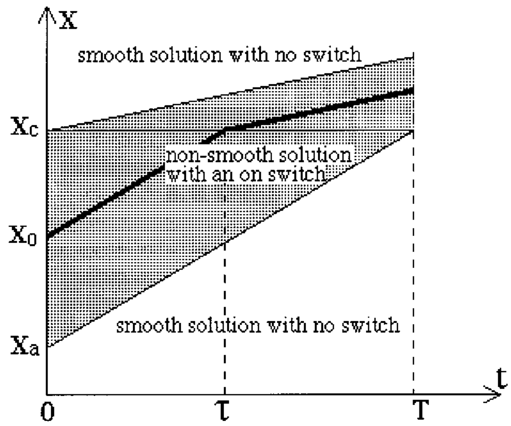

Fig. 1. Initial states and solutions for the analytical example (see case II in subsections 3b and 6b(2) of X96a). The lower thin line is the solution with $x_0 = x_a$ and $\tau = T$. The upper thin line is the solution with $x_a = x_c$ and $\tau = 0$. The thick line in the shaded region shows a non-smooth solution for which the initial state is between $x_a < x_0 < x_c$ and an on switch is triggered within the data assimilation time window $(0, T)$.

necessarily cause discontinuities in the gradient of the costfunction. As shown in Figs. 1, 2 (which partially duplicate Figs. 8, 9 of X96a), when the initial state varies over the range of $x_a \leqslant x_0 < x_c$, the solution contains an on switch within the data assimilation time window ($0 < t \leqslant T$), but the gradient of the costfunction is continuous over the

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Fig. 2. Gradient over the range of the initial states shown in Fig. 1.

range of $x_a \leqslant x_0 < x_c$. Here, the analytical model is described by (2.1) of X96a (or (4.1) of Z97), x_c is the threshold value, and τ denotes the switch time. With an analytical model, the gradient becomes discontinuous (at zero order or higher order) only at those points where the initial state changes the topologic property of the solution (from one type to another). For example, as shown in Fig. 2 (or Fig. 9 of X96a), the gradient becomes discontinuous only when the initial state passes x_c, and thus the solution changes from smooth (with an on switch) to non-smooth (with no switch). When the initial state passes point x_a and the solution changes from non-smooth (with no switch within the time window of $0 < t \leqslant T$) to smooth, the gradient is continuous, but its derivative becomes discontinuous (see Subsection 6b(2) of X96a for the detailed analysis). Other examples can be seen in Figs. 11 and 13 of X96a, where discontinuities in the gradients were caused by the changes of solution's topologic properties at non-bifurcated and bifurcated branch points. Changes of the solution's topologic properties can create discontinuities in the gradient, even in the absence of on–off switch effects. Time-discontinuous on/off switches in the solution and spatial-discontinuities of the costfunction gradient in the parameter space (such as the initial state) are different concepts, and should not be confused with each other.

(b) The Frechet differential and Gateaux differential were introduced in Section 3 of Z96. These generalized derivatives are extensions of the classic gradient and directional derivative for infinite-dimensional spaces. In a finite-dimensional space, such as the space of grid variables in a numerical model, the Frechet derivative is equivalent to gradient and the Gateaux derivative is equivalent to directional derivative. In a one-dimensional space, the Frechet derivative is just the classic derivative and the Gateaux derivative is simply one-sided. Generalizations of the classic gradient and directional derivative are necessary only when the number of dimensions of the concerned space becomes infinitely large. Since the costfunctions in Z97 were all in finite-dimensional spaces, it was not really the case that "a more general definition of the derivative of the costfunction is required to understand the result of adjoint model integration". As far as on–off switches are concerned, what really needs to be generalized is the classic concept of solution. The switch-related step-function does not satisfy the well-known Lipschitiz condition — the condition that insures the existence, uniqueness and continuous dependence of the solution on its initial condition in the classical sense. In order to derive the tangent linear and adjoint equations, it is necessary to extend the classic concept and to describe the solution in terms of a generalized function. This type of extension was introduced with generalized adjoint formulations in X96a, based on the rigorous modern mathematical theory on generalized functions (see, e.g. Appendix to Chapter VI, Courant and Hilbert 1962).

3. Problems in the "practical" linearization that ignores the variation of switch time

The nonlinear solution and related perturbation solution in (4.3)–(4.11) of Z97 are similar to that in (3.4)–(3.6) of X96a, although (q, β) were used in (4.1) of Z97 in place of (x, G) in (2.1) of X96a. While these solutions have the correct forms as in X96a, their derivation was not correctly described in Z97 as it missed the central point. It was described in Z97 that the perturbation solution in (4.10) was derived from (4.3) by "keeping the 'on–off' switch the same as in the NLM". This was not a correct statement, since the switch time $\tau = (q_c - q_0)/F$, was not fixed in the factor, $(t - \tau)$, outside the Heaviside function. The variation of τ outside the heaviside function caused a first-order perturbation, $\tau' = \tau = -q_0'/F$, which was actually included in (4.10)–(4.11). The perturbed solution in (4.4) of Z97 also considered the variation of the switch time (from τ to τ'). Consequently, none of the results in (4.3)–(4.11) of Z97 really "proves that keeping the 'on–off' switches fixed the resulted 'first-order' perturbation solution is correct" (see the text after (4.11) in Z97). As explained in the introduction of X96a, "the variation of the switch point is a leading order perturbation for a discontinuous switch, but this leading order perturbation was ignored in the previous studies". This was one of the major points concerned in X96a. As shown by Figs. 2, 3 in section 3 of X96a (also see Fig. 3 here), the variation of the switch point cannot be ignored, otherwise the resulted perturbation solution (as well as the resulted perturbation equation) will be incorrect in the first-order.

In the same paragraph after (4.11) in Z97, it was also stated that "in the practical TLM and adjoint model development, linearization is carried out for the tendency eq. (4.1) instead of its solution (4.3), result becomes different". As commented above, the direct linearization of the solution in (4.3)–(4.11) of Z97 was actually not the same as the "practical" linearization (that ignored the variation of the switch point); and this explains why "result becomes different". Besides, the "practical" linearization in (4.12)–(4.16) have the following problems.

(a) The "practical" TLM equations (4.12a,b) in Z97 were obtained for the two time periods (before and after the switch) with the switch point fixed. The "initial condition" at $t=\tau$ in (4.12b) was given externally. This required the perturbation solution be known in advance, which contradicted the purpose of using the equation to find the solution. To derive the TLM equation valid for the entire period $[0, T]$ including the switch point, it is necessary to consider the variation of the switch point. As shown in Fig. 3 (partially duplicates Fig. 3 of X96a), the tangent linear perturbation (shaded) differs from the nonlinear perturbation (thin line) only over the time interval of $\delta\tau$. This difference is of high-order, measured by the L_2-norm over $[0, T]$ according to (5.2) of X96a. The jump at the switch point suggests that the resultant TLM equation contains a delta function at the switch point as indicated by the arrow in the lower panel of Fig. 3. This TLM equation can be integrated across the switch point with a jump produced by the delta function (see (3.7) of X96a).

(b) The "practical" adjoint equations (4.13a,b) of Z97 were obtained for the same two time periods as in the TLM equations with the switch point fixed. These adjoint equations were not connected by themselves at the switch point, so they cannot be integrated across the switch point. The correct adjoint equation should be derived from the TLM equation valid for the entire period $[0, T]$ including the switch point, and the derived adjoint equation should also contain a delta function at the switch point (see (3.8) of X96a).

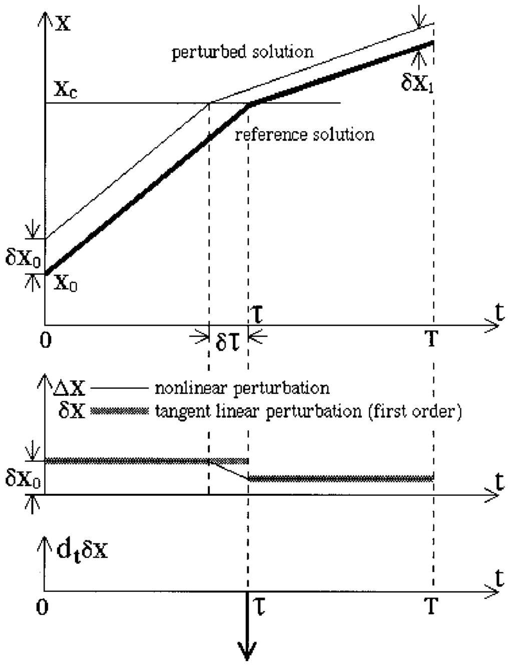

Fig. 3. Upper panel: reference solution (thick line) and perturbed solution (thin line) obtained from equation (2.1) of X96a. Middle panel: nonlinear perturbation (thin line) and tangent linear perturbation (shaded). Lower panel: delta function (arrow at $t=t$) in the TLM.

(c) The first-order variation in (4.15)–(4.16) of Z97 was derived by keeping the switch fixed. The last term required that the dependence of the perturbation solution at $t=\tau$ (after the switch) on the initial perturbation (at $t=0$) be known in advance or, say, the gradient of the solution at $t=\tau$ (after the switch) with respect to the initial state be known in advance. This contradicted the purpose of using the adjoint to find the gradient. The correct variation of the costfunction should consider the variation of the switch point and the result should be the inner product of the TLM perturbation and adjoint solution at the initial time only (see (4.7) of Xu (1996b)).

All the above-mentioned problems are also seen in (4.25)–(4.31) of Z97.

4. Problems with applicability of the "practical" linearization

The equation and solution in (4.35)–(4.37) of Z97 are similar to that in (7.1)–(7.3) of X96a. Based on these results, the continuity of the TLM solution was proposed in (4.38) of Z97 as a sufficient condition for the applicability of the "practical" linearization. Since this condition is simply related to the continuity of the forcing term in the original model equation, it should be straightforward to consider the latter (see Subsection 3, 7 and 8 of X96a).

In Z97, (4.40) was used to modify the last variable in (4.17), and the purpose was to make the right-hand-side of the tendency equation (4.17) continuous in time at the switching point. Note that the right-hand-side of (4.40) takes the non-zero threshold value at the switch point as assumed in Z97, so the last term in the modified (4.17) should be given by $H(q-q_c)\alpha(q_c+$higher-order small terms) which is still discontinuous at the switch point. While this error could be easily corrected with the jump in (4.17) of Z97 fitted by a linear function of time as in (7.6) of X96a, the variation of switch time cannot be ignored. Thus, there is no real proof for the statements in the two paragraphs after (4.40) in Z97. In particular, one cannot see why "the TLM and adjoint model developed assuming that all 'on–off' switches are determined by the unperturbed NLM solution may still provide a correct first-order information", and how "constructing the adjoint model at the coding level" could avoid the problem caused by on–of switches in the "practical" linearization. In the contrary, the recent studies of Xu (1997) and Xu et al. (1998) indicate that problems caused by the variation of switch time in a time-discretized model cannot be correctly treated by the "practical" linearization, but the problems can be solved by using the generalized adjoint.

5. Acknowledgment

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