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Application of the complex step method to chemistry-transport modeling

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HIGHLIGHTS

- Sensitivity analysis is widely used in chemistry-transport modeling.
- The common finite difference approach incurs numerical errors.
- We implement the complex step in a chemistry-transport for the first time.
- The method results in near-exact sensitivities and is straightforward to implement.
- We also propose a combined complex step/adjoint approach.

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ABSTRACT

Sensitivity analysis in atmospheric chemistry-transport modeling is used to develop understanding of the mechanisms by which emissions affect atmospheric chemistry and composition, to quantify the marginal impact of emissions on air quality, and for other applications including improving estimates of emissions, developing fast first order air quality models, and validating adjoint models. Forward modeling sensitivities have predominantly been calculated using the finite difference approach, i.e. where the results of two separate simulations are subtracted. The finite difference approach incurs truncation and cancellation errors, which mean that exact sensitivities cannot be calculated and even approximate sensitivities cannot always be calculated for a sufficiently small perturbation (e.g. for emissions at a single location or time). Other sensitivity methods can provide exact sensitivities, but require the reformulation of non-linear steps (e.g. the decoupled direct method) or the development of adjoints of entire codes (partly automatically and partly manually). While the adjoint approach is widely applied and has significant utility in providing receptor-oriented information, in some applications the source-oriented information of forward approaches is needed. Here we apply an alternative method of calculating sensitivities that results in source-oriented information as with the finite difference approach, requires minimal reformulation of models, but enables near-exact computation of sensitivities. This approach – the complex step method – is applied for the first time to a complete atmospheric chemistry-transport model (GEOS-Chem). (The complex step method has been previously used in validating the adjoint of an aerosol thermodynamic equilibrium model.) We also introduce the idea of combining complex-step and adjoint sensitivity analysis (for the first time in any context to our knowledge) to enable the direct calculation of near-exact second order sensitivities.

1. Introduction

Sensitivity analysis is the study of how the outputs of a model are affected by changes in the values of the inputs (Morgan and Henrion, 1990). In the context of atmospheric chemistry-transport models (CTMs), this typically entails computing the change in a species concentration with respect to a change in a species emission. The EPA recommends that sensitivity analysis be used early and often in the development and validation of computational models of the environment (EPA, 2009). Sensitivity analysis is also applied in the development of rapid surrogate models of more complex CTMs and in the analysis of potential air

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quality policies (e.g. Ashok et al., 2013). It is used both in determining which model parameters can be excluded from a particular class of problem (due to relatively low sensitivity), and for developing the parameters used by surrogate models. Sensitivity analysis is used in combination with uncertainty analysis to attribute uncertainty in outputs of models to uncertainty in their inputs (Beck et al., 1994). This informs users on the confidence that can be placed in models.

1.1. Sensitivity methods implemented in CTMs

The major classes of sensitivity methods implemented in CTMs are 1) the finite difference (FD) method, 2) the adjoint method, 3) the decoupled direct method (DDM), and 4) the Green's function method (GFM).

The FD method is the most common sensitivity method used with CTMs because it is relatively straightforward to implement (van Keulen et al., 2005). The FD method in CTMs has been extensively used in climate and air quality sensitivity problems (Fry et al., 2012; Kohler et al., 2008; Naik et al., 2005; Stevenson et al., 2004) as well as in validating the implementation of the adjoints, e.g. GEOS-Chem (Henze et al., 2007).

The FD method is based on running a CTM twice: one simulation to obtain the reference results and another simulation with a perturbed input variable. The two results are then post processed to obtain sensitivities. The FD approximation is given by.

$$f'(x_0) \cong \frac{f(x_0+\Delta)-f(x_0)}{\Delta}, \quad (1)$$

where x_0 is the reference value of the input variable and Δ is the perturbation. Relating to CTMs, f is the result of the CTM (e.g. the concentration of a chemical species at a location), x_0 is an input to the CTM (e.g. an emission) and $f'(x_0)$ is the sensitivity of the result with respect to the input.

A drawback of the FD method is that there is a tradeoff between truncation and cancelation errors (Martins et al., 2003; Squire and Trapp, 1998; van Keulen et al., 2005). The truncation error is associated with non-linearity (i.e. ignoring the higher order terms) and is reduced by decreasing Δ. However, at some decrease in Δ the cancelation error increases because, in finite precision, the reference and perturbed results become indistinguishable (resulting in "noisy" results). In practice this limits the calculation of sensitivities in CTMs to sufficiently large perturbations, which may be of a magnitude to incur truncation errors depending on the non-linearity of the specific problem.

The DDM has been used in computing first order sensitivities in air quality models (Dunker et al., 2002) and higher order sensitivities (HDDM, Hakami et al., 2003, 2004). The DDM method and the adjoint method are similar because they are both derived by differentiating the original code (i.e. algorithm differentiation) of the model and both produce near-exact sensitivities. The difference is that the DDM is a forward sensitivity method and the adjoint is a reverse method. The DDM method entails reformulating and recoding the extensive parts of the model in which non-linear responses can occur (e.g. chemistry and advection), because equations for sensitivities have different forms to those for concentrations in these cases.

The GFM has been used by Vuilleumier et al. (1997) to study the temporal dependence of O_3 concentrations on the NO_x concentrations. The GFM was designed to be a fast sensitivity analysis method (Rabitz et al., 1983), although it incurs numerical errors and errors that are introduced by the choice in step size (Vuilleumier et al., 1997), similar to the FD method. The GFM is not in widespread use.

The adjoint method is based on differentiation of the forward code and then integration of the sensitivities backwards. This results in computing the sensitivity of one output of the CTM with respect to all the inputs by performing one run of the adjoint model. This has significant utility in applications where many inputs are assessed relative to their impact on one output, such as determining the spatiotemporal locations where emissions reductions result in the greatest total population exposure to a pollutant. Adjoint approaches are not useful where the distribution of impacts from an emissions change is required.

The adjoint method in GEOS-Chem has been implemented by Henze et al. (2007) and has been extensively used in air quality and climate studies (Henze et al., 2012; Bowmann and Henze, 2012; Gilmore et al., 2013; Koo et al., 2013). As a particular example, Turner et al. (2012) used the adjoint sensitivity method in GEOS-Chem to estimate the impact on concentrations due to contributions of local versus distant emissions. The adjoint of GEOS-Chem is a combination of continuous and discrete adjoint code created by both manually implementing the code and by use of automatic adjoint generating tools such as Tangent and Adjoint Model Compiler (TAMC, Giering and Kaminski, 1998), the Kinetic PreProcessor (KPP, Sandu et al., 2003; Damian et al., 2002; Daescu et al., 2003).

A benefit of an adjoint approach is that the sensitivities can be exact. As it is currently implemented, the adjoint of GEOS-Chem can compute sensitivities with respect to scaling factors of emissions, absolute values of emissions, initial concentrations and (more recently) reaction rate constants (GEOS-Chem Adjoint User's Guide (gcadj.v35)). The main drawback of the adjoint is that "the practical implementation of this approach can be challenging" (Giles and Pierce, 2000). Also, because it is based on the forward code it means that for each update and further development of the forward model, the adjoint code must be updated accordingly to reflect the changes in the forward model. Both of these drawbacks are similar to the DDM approach. The adjoint approach also provides receptor-oriented information, which is advantageous in some applications while there are others where source-oriented information (as provided with the FD method) is needed.

1.2. Motivation for the complex step method

As has been described above, forward methods provide information on the spatiotemporal distribution of the impact and not information on the spatiotemporal distribution of the sources. In contrast, adjoint methods provide information on the spatiotemporal distribution of the sources and not information on the spatiotemporal distribution of the impact. Depending on whether the required result of the sensitivity analysis is a spatiotemporal distribution of impacts or a spatiotemporal distribution of sources, one may need to perform a forward sensitivity analysis, a reverse sensitivity analysis or both. Because of this, in CTMs such as GEOS-Chem, adjoint sensitivity methods and forward sensitivity methods can be considered complements of each other and therefore there is need for both. However, while the adjoint method results in exact computation of receptor-oriented sensitivities, there is no accurate way of calculating source-oriented sensitivities in GEOS-Chem, and the exact DDM (applied to CMAQ, for example) incurs the drawbacks of reformulating and rewriting significant portions of the code.

There have also been studies that highlight the importance of computing second order sensitivities. Hakami et al. (2004) states that "addition of higher-order information to the analysis allows more reliable prediction of the response beyond its linear range, particularly when nonlinear behavior is expected". For example,