ON THE APPLICATIONS OF THE ADJOINT SENSITIVITY ANALYSIS TO ASSIMILATION OF *EOS CHEM* LEVEL 3 PRODUCTS

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- Remote sensing and data assimilation: Similarities in goals, tools, and approaches
- Data assimilation: Existing approaches
- Linearization of existing models
- Adjoint sensitivity analysis
- Conclusion

Remote sensing and data assimilation: Similarities in goals, tools and approaches

Goals

Remote sensing: Retrieving the fields of atmospheric parameters (temperatures, VMRs) from observed radiances

Data assimilation: Retrieving the fields of model parameters (surface fluxes, rates of processes, etc.) from fields of atmospheric parameters

Tools

Remote sensing: Theory and applications of radiative transfer

Data assimilation: Theory and applications of atmospheric dynamics and photochemistry

Approaches

Remote sensing: Modeling (rarely); evaluation of sensitivities (jacobians, weighting functions) and inversion of data (in most of applications)

Data assimilation: Modeling (in majority of applications); evaluation of sensitivities (jacobians, weighting functions) and inversion of data (still less frequently)

Data assimilation

Given: Observed state of the atmosphere (fields of atmospheric parameters) and some starting estimates of model parameters

Find: Refined estimates of model parameters

Existing approaches

Modeling:

Nonlinear zero–D, 1D and multi–D models: simulation of the observed state of the atmosphere; model–fitting of observed atmospheric fields by variating (manual or automated) of the model parameters

Forward sensitivity analysis:

Linearized models: simulations of responses of the observed state of the atmosphere to variations of model parameters; yield sensitivities of all observables to a single model parameter; the models are run for each parameter variation separately

Adjoint sensitivity analysis:

Adjoint models (uniquely derived from the linearized models): yield sensitivities of a single observable (usu. cost function) to all model parameters

Inversion of atmospheric fields

Sensitivities obtained using sensitivity analysis algorithms are used as jacobians in corresponding inverse problems

Linearization of photochemical models

Existing photochemical models include many tens, even hundreds of processes and differential equations associated with them, Thus, the linearization needs to be automatized. To do that, the initial system of differential equations is rewritten in the form:

$$\dot{x}_i + \sum_{j,k=1}^{n} A_{jk}^{(i)} x_j x_k + \sum_{j=1}^{n} B_{ij} x_j = S_i^{(0)}$$

$$i = 1, \dots n$$

Here:

x_i – concentrations of 'unknown' atmospheric constituents, that are dependent on model parameters)

$A_{ij}^{(i)} x_i x_j$ – terms due to processes of production and losses of given x_i involving two 'unknown' atmospheric constituents

$B_{ij} x_j$ – terms due to processes of production and losses of given x_i involving one 'unknown' atmospheric constituent

$S_i^{(0)}$ – terms due to processes of production and losses of given x_i involving 'known' constituents only

The above system can be linearized in the form (initial conditions added):

$$\frac{d\mathbf{x}'}{dt} + \mathsf{C}\mathbf{x}' = \mathbf{S}'$$

$$\mathbf{x}'|_{t_0} = \mathbf{x}_0$$

where:

$$C_{ij} = \sum_{k=1}^{n} (A_{jk}^{(i)} x_k + A_{kj}^{(i)} x_k) + B_{ij}$$

$$S_i' = (S_i^{(0)})' - \sum_{j=1}^{n} (B_{ij})' x_j - \sum_{j,k=1}^{n} (A_{kj}^{(i)})' x_j x_k$$

Adjoint sensitivity analysis

Evaluation of linearized observables $\mathbf{R}'$ using two approaches:

Forward approach: Solve the linearized forward problem:

$$\frac{d\mathbf{x}'}{dt} + \mathsf{C}(t)\,\mathbf{x}'(t) = \mathbf{s}_e(t)$$

$$\mathbf{x}'\big|_{t_0} = \mathbf{s}_c$$

and convolve the observables:

$$\mathbf{R}' = \int_{t_0}^{t_1} \mathsf{W}_e(t)\,\mathbf{x}'(t)\,dt + \mathsf{W}_c\,\mathbf{x}'(t_1)$$

Adjoint approach: Solve the adjoint problem:

$$-\frac{d\mathsf{X}^*}{dt} + \mathsf{C}^{\mathsf{T}}(t)\mathsf{X}^*(t) = \mathsf{W}_e^{\mathsf{T}}(t)$$

$$\mathsf{X}^*\big|_{t_1} = \mathsf{W}_c^{\mathsf{T}}$$

and convolve the observables:

$$\mathbf{R}' = \int_{t_0}^{t_1} \mathsf{X}^*(t)\,\mathbf{s}_e(t)\,dt + \mathsf{X}^*(t_0)\,\mathbf{s}_c$$

Evaluation of sensitivities to model parameters p_k:

Forward approach:

$$\frac{\partial \mathbf{R}}{\partial p_k} = \int_{t_0}^{t_1} \mathsf{W}_e(t)\,\frac{\partial \mathbf{x}}{\partial p_k}\,dt + \mathsf{W}_c\,\frac{\partial \mathbf{x}}{\partial p_k}\bigg|_{t_1}$$

Adjoint approach:

$$\frac{\partial \mathbf{R}}{\partial p_k} = \int_{t_0}^{t_1} \mathsf{X}^*(t)\,\frac{\partial \mathbf{s}_e}{\partial p_k}\,dt + \mathsf{X}^*\bigg|_{t_1}\frac{\partial \mathbf{s}_c}{\partial p_k}$$

NB: the adjoint approach needs a *single* adjoint solution.

Conclusion

• Existing nonlinear models of assimilation of Level 3 products can be linearized by relatively moderate amount of effort (as compared to building the nonlinear models themselves).

• Resulting linearized models give an opportunity to do the sensitivity analysis easing the process of data assimilation; the need to do one run per parameter still presents a computational burden.

• Adjoint models derived from the linearized models give further opportunities to do the sensitivity analysis with respect to all model parameters simultaneously.

• Computed sensitivities of observables to the model parameters can be used for inversion of Level 3 data in terms of refined estimates of model parameters defining the sources and sinks of observed constituents.