A prototype of a data assimilation system based automatic differentiation

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Overview

- Calibration step
- Prognostic step
- Model development within system
- Automatic Differentiation
- Summary
Setup for Calibration Step

Parameters: 57

**Biosphere Model: BETHY**

Fluxes: 10'000 per year

Background Fluxes

**Atmospheric Transport Model: TM2**

Concentrations: 500 per year

Observations

J

Misfit: 1

**BETHY: Knorr 97; TM2: Heimann 95**
Gradient Method

First derivative (Gradient) of $J(m)$ w.r.t. $m$ (model parameters):

$$-\frac{\partial J(m)}{\partial m}$$

yields direction of steepest descent

Figure taken from Tarantola '87
CO$_2$ concentration at station Alert

- first guess
- observed

Year

CO$_2$ [ppm]


420

400

380

360

340

320
CO₂ concentration at station Alert

- observed
- optimised

Year

CO₂ [ppm]
320 340 360 380 400 420

Optimisation
Optimisation
Optimisation

CO₂ concentration at station Alert
- observed
- optimised

CO₂ concentration at station wis (red: observed)
Optimisation
CO₂ concentration at station Alert

- observed
- optimised

CO₂ concentration at station spo (red: observed)
Covariances in Parameter Uncertainties

Second Derivative (Hessian) of $J(m)$:

$$\frac{\partial^2 J(m)}{\partial m^2}$$

yields curvature of $J$, provides estimated uncertainty in $m_{opt}$

Figure taken from Tarantola '87
Covariances in Parameter Uncertainties

Second Derivative (Hessian) of $J(m)$:

$$\frac{\partial^2 J(m)}{\partial m^2}$$

yields curvature of $J$, provides estimated uncertainty in $m_{\text{opt}}$

Figure taken from Tarantola '87

Space of $m$ (model parameters)
Covariances in Parameter Uncertainties

Cost function (misift):

\[ J(r_m) = \frac{1}{2} [r_m - r_{m_0}] C_m^{-1} [r_m - r_{m_0}] + \frac{1}{2} [y(r_m) - y_{0}] C_y^{-1} [y(r_m) - y_{0}] \]

- Assumed model parameters
- A priori parameter values
- A priori covariance matrix of parameter uncertainty
- Model prediction
- Measurements
- Covariance of uncertainty in measurements + model
Covariances in Parameter Uncertainties

Cost function (misift):

\[ J(m) = \frac{1}{2} [r_m - r_{m_0}] C_{m_0}^{-1} [r_m - r_{m_0}] + \frac{1}{2} [y(m) - y_{0}] C_{y}^{-1} [y(m) - y_{0}] \]

Covar. of parameter uncertainties after optimisation:

\[ C_m = \left\{ \frac{\partial^2 J}{\partial m_i \partial m_j} \right\}^{-1} = \text{inverse Hessian} \]
Covariances in Parameter Uncertainties

Cost function (misift):

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Covar. of parameter uncertainties after optimisation:

\[ C_m = \left\{ \frac{\partial^2 J}{\partial m_i \partial m_j} \right\}^{-1} = \text{inverse Hessian} \]

Examples:

<table>
<thead>
<tr>
<th></th>
<th>first guess</th>
<th>optimized</th>
<th>prior unc.</th>
<th>opt.unc.</th>
<th>Vm(TrEv)</th>
<th>Vm(EvCn)</th>
<th>Vm(C3Gr)</th>
<th>Vm(Crop)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \mu \text{mol/m}^2 \text{s} )</td>
<td>( \mu \text{mol/m}^2 \text{s} )</td>
<td>%</td>
<td>%</td>
<td>\mu mol/m \text{s}</td>
<td>\mu mol/m \text{s}</td>
<td>%</td>
<td>%</td>
</tr>
<tr>
<td>Vm(TrEv)</td>
<td>60.0</td>
<td>43.2</td>
<td>20.0</td>
<td>10.5</td>
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<td>0.05</td>
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<tr>
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<td>-0.10</td>
<td>0.08</td>
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<td>18.0</td>
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<td>16.9</td>
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<td>Vm(Crop)</td>
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<td>45.4</td>
<td>20.0</td>
<td>17.8</td>
<td>0.05</td>
<td>0.08</td>
<td>-0.31</td>
<td>0.80</td>
</tr>
</tbody>
</table>
Relative reduction of uncertainties

Observations resolve about 10-15 directions in parameter space
Setup for prognostic step

- Parameters: 57
- Biosphere Model: BETHY
  - Fluxes: 10'000 per year
  - Atmospheric Transport Model: TM2
    - Prognostic Concentrations
    - Prognostic Fluxes
      - Background Fluxes
        - Parameter: 1

BETHY: Knorr 97; TM2: Heimann 95
Covariance in uncertainties of prognostics, $y$, after optimisation (e.g. CO$_2$ fluxes):

$$
C_y(r_{m_{opt}}) = \left( \frac{\partial y_i(m_{opt})}{\partial m_j} \right) \cdot \left( \begin{array}{c} \frac{\partial y_i(m_{opt})}{\partial m_j} \\ \vdots \end{array} \right)^T
$$

Jacobian matrix (adjoint or tangent linear model)

Error covariance of parameters
Regional Net Carbon Balance and Uncertainties

Carbon Flux (MtC/year)

- Europe
- North-America
- Russia
- Brazil
- Australia

Legend:
- Biospheric Carbon Sink
- Fossil Fuel Emissions
- Landuse Change Emissions
Regional Net Carbon Balance and Uncertainties

![Graph showing carbon flux (MtC/year) for different regions: Europe, North-America, Russia, Brazil, and Australia. The graph includes bars for biospheric carbon sink, fossil fuel emissions, and land use change emissions.](image-url)
Model development within System

- System can test a given combination observational data + model formulation with uncertain parameters, and deliver optimal parameters, prognostics, and their a posteriori uncertainties
- Model is developed further within system
- Model development benefits from sensitivity information and comparison with data (often brutal!)
- Work is ongoing, numbers are from model formulation we are not yet happy with...
Automatic Differentiation

- Uses adjoint, tangent linear and Hessian code
- All this derivative code generated from F90 source code of model (~5500 lines) by automatic differentiation tool TAF
- CPU time in multiples of model (on Linux: 2 XEON 2GHz):
  - tangent linear: 2.1
  - adjoint: 3.4
  - Hessian * 12 vectors: 50
Summary

• Concept can be generalised to other modeling systems, e.g.
  -> Ocean: MIT model, presentation of Heimbach et al.
  -> NWP: DAO fvGCM, poster Giering et al.

• Automatic differentiation helps to reduce the delay from model development to data assimilation