On the Estimation of Posterior Error Bars

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Introduction

Posterior error estimates are important parts of an inverse method solution. Unfortunately, their evaluation can become computationally quite demanding since this task always involves some sort of inverse of the Hessian of the problem. However, some observables for which the error estimates are required can be represented by a relatively small part of the Hessian spectrum and thus do not need its full inverse for estimating their errors.

We propose a polynomial approximation of the Hessian spectrum which enables us to obtain reliable error estimates for some observables. We compare the results to “standard” methods and show examples of applications for large problems.

Methods

1. Full inversion

The inverse of the Hessian of the cost function is the covariance of the deviation of the control variables \( \phi \) from the optimal state \( \phi^* \). An observable \( \Phi_\alpha \) \( \alpha=1,2,... \) can be expanded into powers of \( \phi - \phi^* \):

\[
\Phi_\alpha = \Phi_\alpha(\phi^*) + \phi_\alpha(\phi - \phi^*) + \ldots
\]

One finds that near the optimum state the covariance of the observables can be approximated as \( \hat{\Phi}_\alpha = \Phi_\alpha(\phi^*) \).

2. Conjugate gradients

When the dimension \( D \) of the problem is very large, it is still possible to calculate the vector \( H\phi \) for any \( \phi \). In order to find \( \hat{\Phi}_\alpha \), the equation \( H\phi = \Phi_\alpha \) is solved for \( \phi \) with a conjugate gradients method to obtain the covariance \( \hat{\Phi}_\alpha \).

3. Polynomial Approximation

The covariance \( \hat{\Phi}_\alpha = \Phi_\alpha(\phi^*) \) is written in a more symmetric form \( \hat{\rho}_{\alpha\beta} \) with \( \Phi = H^{1/2} \phi \) as

\[
\hat{\rho}_{\alpha\beta} = \frac{1}{2} \sum_{i=1}^{D} \frac{\delta(H) \delta_\alpha \delta_\beta}{\delta(H)}(\phi_i^*)^2
\]

with \( \phi_i = U_i/\sqrt{2} \delta_\alpha \delta_\beta \). Truncation of the series corresponds to smoothing the spectrum of the Hessian \( H \). Let \( \phi_i = \sin(i\pi/2) \) be the eigenvectors of \( H \) and \( \epsilon_i \) the eigenvalues, then the spectral function is

\[
\hat{\rho}_{\alpha\beta} = \frac{1}{D} \sum_{i=1}^{D} \frac{\delta(H) \delta_\alpha \delta_\beta}{\delta(H)}(\phi_i^*)^2
\]

is the spectral function of the Hessian \( H \), weighted by \( \phi_i^* \). Truncation results again in smoothing the spectrum. From this spectrum we can decide what part of the spectrum of \( H \) is needed for the correct evaluation of \( \hat{\rho}_{\alpha\beta} \).

4. Comparison

For the Southern Ocean WOCE section SR3 a small geostrophic toy model with 136 control variables (tracers and bottom velocities) illustrates the three methods described. Figures 1 and 2 show the temperature and velocity field after inversion. The posterior errors and their correlation of the total mass and heat transports through the section obtained by the three different methods show a reasonable agreement (Table 1).

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<tr>
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<tbody>
<tr>
<td>Full inversion</td>
<td>520</td>
<td>32</td>
<td>1.7</td>
<td>0.17</td>
</tr>
<tr>
<td>Conjugate gradients</td>
<td>500</td>
<td>32</td>
<td>1.7</td>
<td>0.28</td>
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<td>Polynomial</td>
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</table>

Figure 1: Temperature of toy model for SR3. Note the coarse grid.

Figure 2: Velocity normal to section (cm/s) of the toy model of SR3.

Figure 3: Hessian matrix of the toy model

Figure 4: Eigenvaluespectrum of the Hessian matrix of the toy model. The condition number is 3x10^6

Figure 5: Same eigenvaluespectrum of the Hessian matrix of the toy model for SR3 as in Figure 4. The representation has been changed to match that of figures 6-8 (lower panels). On the abscissa, there are the normalized magnitude of the eigenvalues, on the ordinate the index number of the eigenvalues relative to the dimension of the problem \( D = 136 \).
Examples of Applications

1. Box model of the Southern Ocean

An inverse box model of the Southern Ocean estimates heat and volume fluxes per layer through hydrographic sections. The control space has 1000 dimensions. This makes the full inversion of the Hessian possible. As an example of the results, the mass flux and flux errors for the zonal Indian Ocean section along 32°S (November) are shown in Figure 9. Table 2 lists the correlation of the flux errors of the different water masses

Table 2: Correlation of mass flux errors for Indian 32°S (SW = Surface/Thermocline Water, IW = Intermediate Water, ULDW = Upper/Lower Deep Water, BW = Bottom Water)

<table>
<thead>
<tr>
<th></th>
<th>SW</th>
<th>TW</th>
<th>UDW</th>
<th>LDW</th>
<th>BW</th>
</tr>
</thead>
<tbody>
<tr>
<td>SW</td>
<td>0.95</td>
<td>0.07</td>
<td>0.06</td>
<td>0.13</td>
<td>0.21</td>
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<td>TW</td>
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<td>0.13</td>
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<td>UDW</td>
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<td>1</td>
<td>0.13</td>
<td>0.09</td>
</tr>
<tr>
<td>LDW</td>
<td>0.05</td>
<td>0.09</td>
<td>0.04</td>
<td>1</td>
<td>0.59</td>
</tr>
<tr>
<td>BW</td>
<td>0.21</td>
<td>0.05</td>
<td>0.07</td>
<td>0.89</td>
<td>1</td>
</tr>
</tbody>
</table>

2. Nonlinear section inverse -- a twin experiment

A nonlinear geostrophic inverse model similar to the one used as the toy model (see above) is applied to the meridional Southern Ocean WOCE section SR3 between Tasmania and the Antarctic continent, to estimate mass and property transports. As the number of control variables is quite large (~17000), the Hessian cannot be calculated nor inverted explicitly. The errors in Table 3 are estimated using the conjugate gradients approach, where for each variance estimate several thousand iterations were necessary for the algorithm to converge.

Table 3: Transport estimates through SR3

<table>
<thead>
<tr>
<th></th>
<th>Mass (10^6 m^3/s)</th>
<th>Heat (PW)</th>
<th>Salt (10^1 µmol/kg)</th>
<th>Oxygen (µmol/l)</th>
<th>Silicate (10^1 µmol/kg)</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>146 x± 29</td>
<td>1.72 x± 0.33</td>
<td>50 x± 10</td>
<td>54 x± 7</td>
<td>84x±25</td>
</tr>
</tbody>
</table>

3. Nonlinear section inverse -- a twin experiment

The same model in the previous section but augmented with satellite altimetry data is used to invert an artificial hydrographic section data set produced by a general circulation model (1/12° North Atlantic Model of the FLAME group). The zonal section is located in the North Atlantic along 24.5°N. Again the number of control variables is fairly large (~12000) and the Hessian cannot be computed completely. Here for the variance estimation of the mass and heat transports, the polynomial approximation approach is employed. Figure 10 and 11 show the spectral density of the Hessian of the model and the weighted spectral density for mass and heat transports through one small part of the section (Florida Strait). Note that the number of coefficients used to represent the Hessian spectrum is not larger than for the toy model, although the problem is much larger, neither does the number of coefficients needed for the inversion depend directly on the dimension of the problem. The transports and errors obtained by this method are for mass 28.2 x± 8.5 µSv and for heat 2.35 x± 0.57. The correlation is 0.87.

Conclusions

Three methods are presented for the calculation of posterior errors of inverse solutions. Of these methods, the full inversion of the Hessian is the most accurate but it is only applicable to small and moderate size problems. One of the other methods the conjugate gradient approach leads to reliable results, but is computationally more expensive than finding the solution of the inverse problem itself. The polynomial approximation on the other hand yields also reliable estimates of the errors, but it involves an approximation of the Hessian spectrum by Chebyshev’s Polynomial. This drawback is at the same time a great advantage over the conjugate gradient method because it decreases computing time by an order of magnitude.

References