A trust region approach to optimal estimation in atmospheric retrievals

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Non-linear Least Squares (NLLS) Optimization

Two algorithms are considered for minimizing the cost functions posed by ML and MAP. They both linearize the forward model:

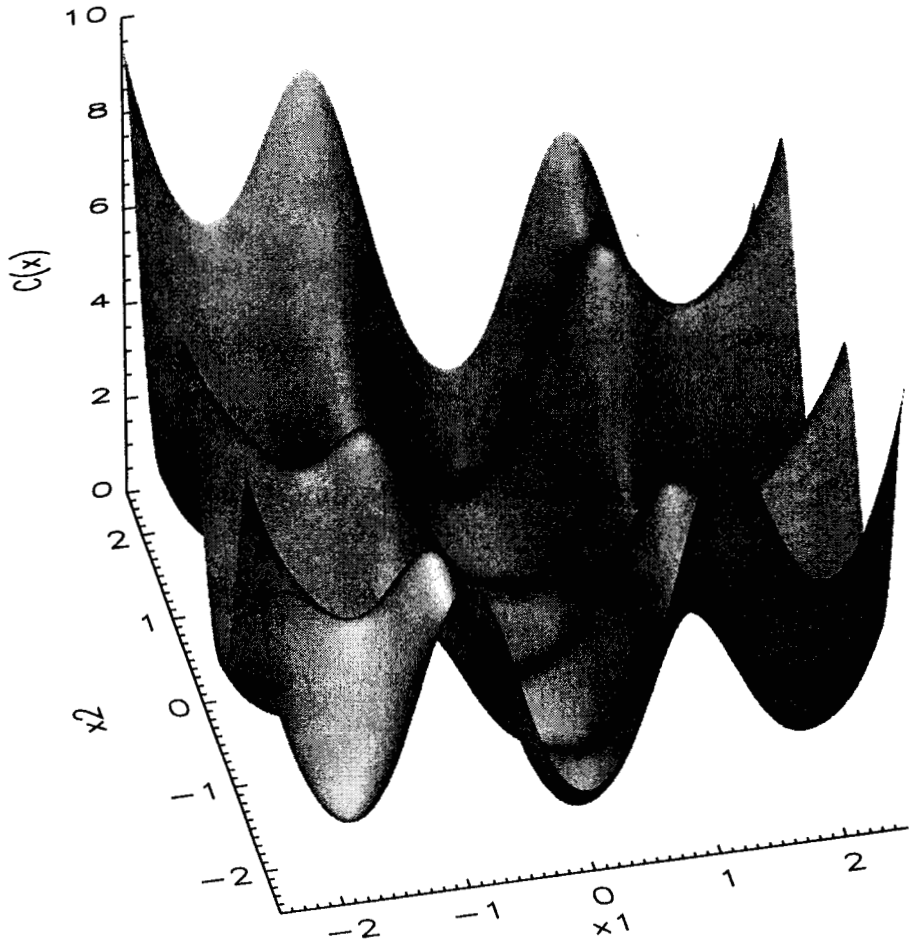
$$\mathbf{F}(\mathbf{x}_{i+1}) \approx \mathbf{F}(\mathbf{x}_i) + \mathbf{K}\delta\mathbf{x},$$

which leads to

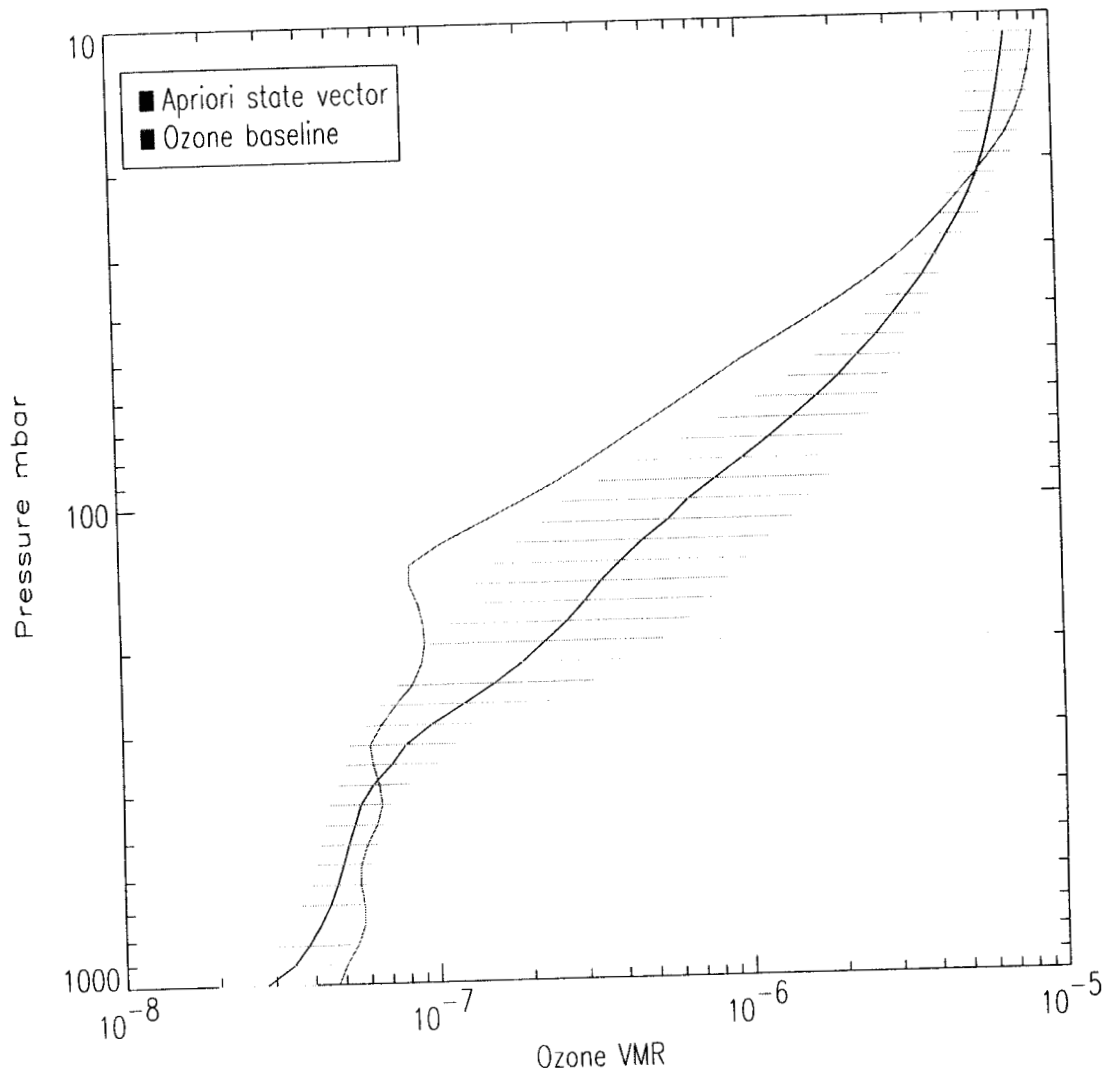
$$\underbrace{\begin{bmatrix} \mathbf{S}_e^{-1/2}\mathbf{K} \\ \cdots \\ \mathbf{S}_a^{-1/2} \end{bmatrix}}_{\mathbf{K}'} \delta\mathbf{x} = \underbrace{\begin{bmatrix} -\mathbf{S}_e^{-1/2}(\mathbf{y} - \mathbf{F}(\mathbf{x}_i)) \\ \cdots \\ \mathbf{S}_a^{-1/2}(\mathbf{x}_i - \mathbf{x}_a) \end{bmatrix}}_{\mathbf{r}} \begin{matrix} ML \\ \cdots MAP \end{matrix}$$

where $\mathbf{K} = \frac{\partial \mathbf{F}}{\partial \mathbf{x}} \in \mathbb{R}^{N \times M}$ is the Jacobian, and $\delta\mathbf{x} = \mathbf{x}_{i+1} - \mathbf{x}_i$.

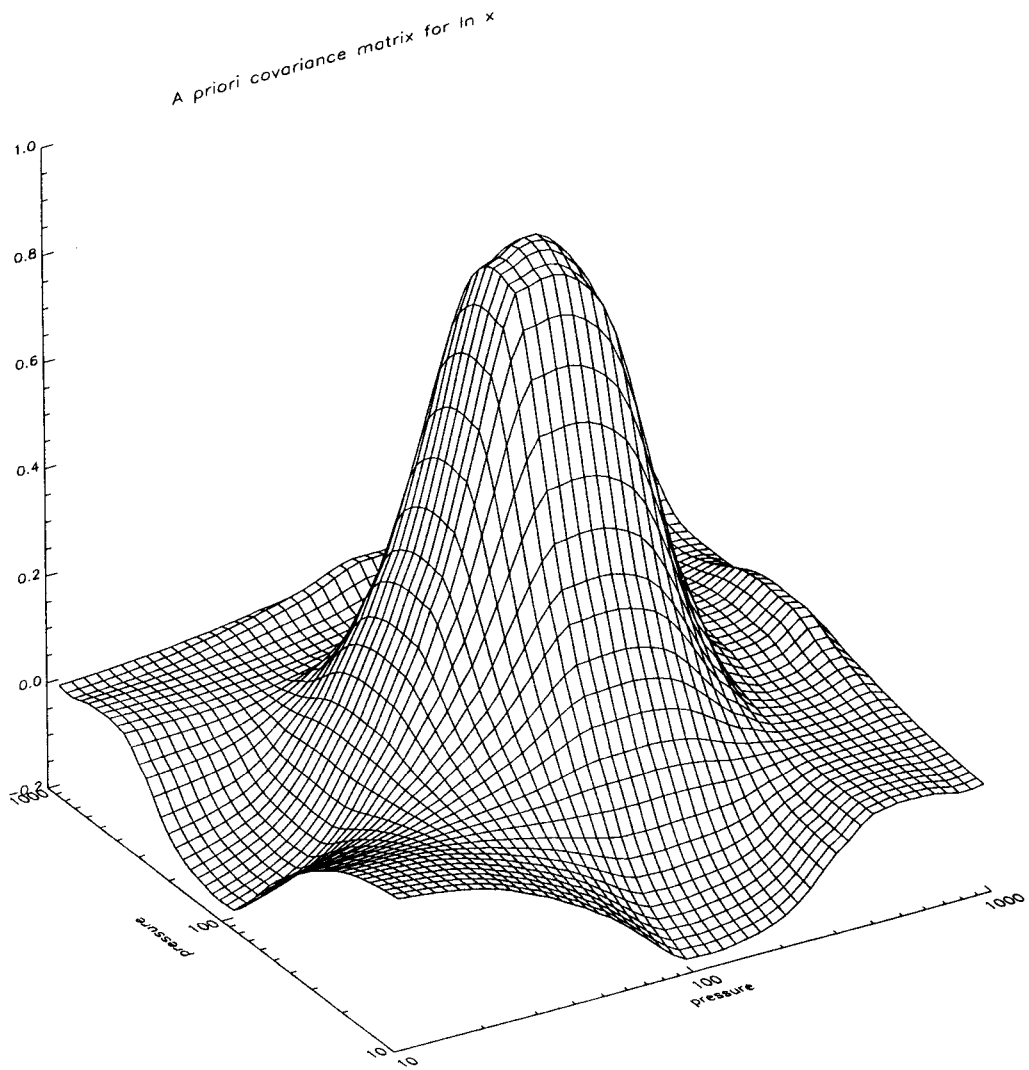
Example Cost Function



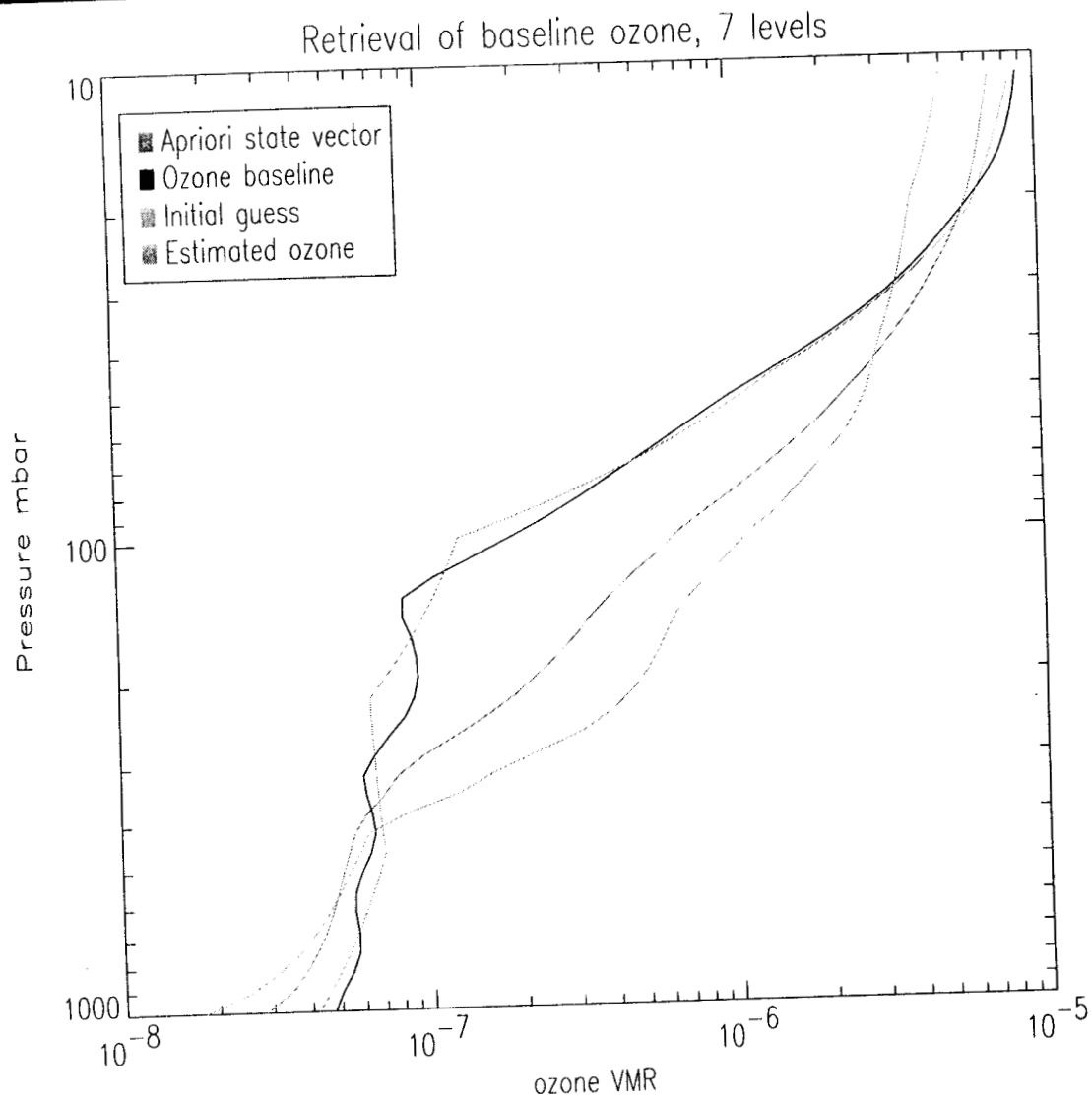
A priori state vector and baseline ozone

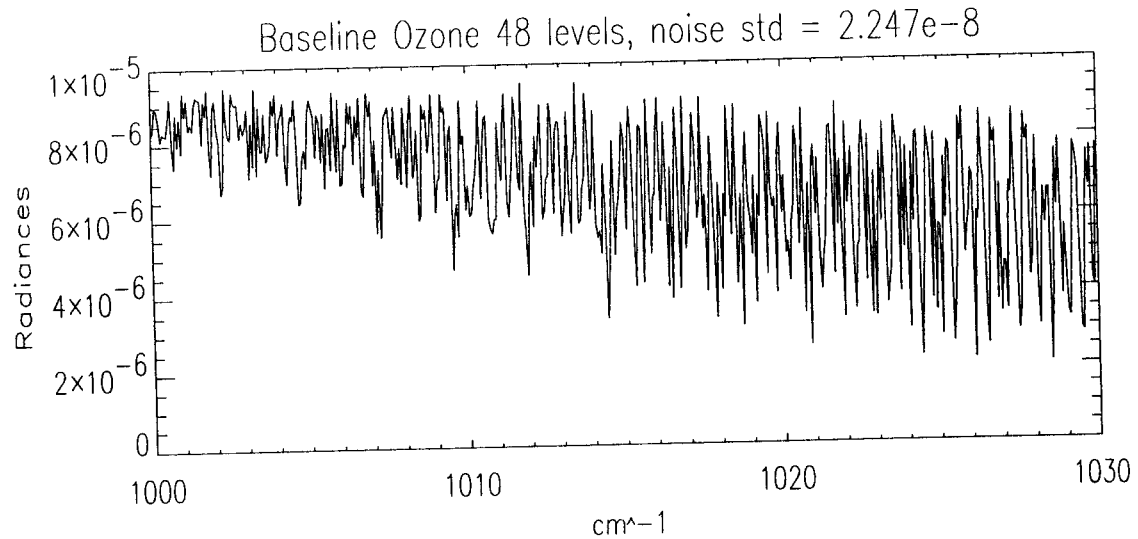


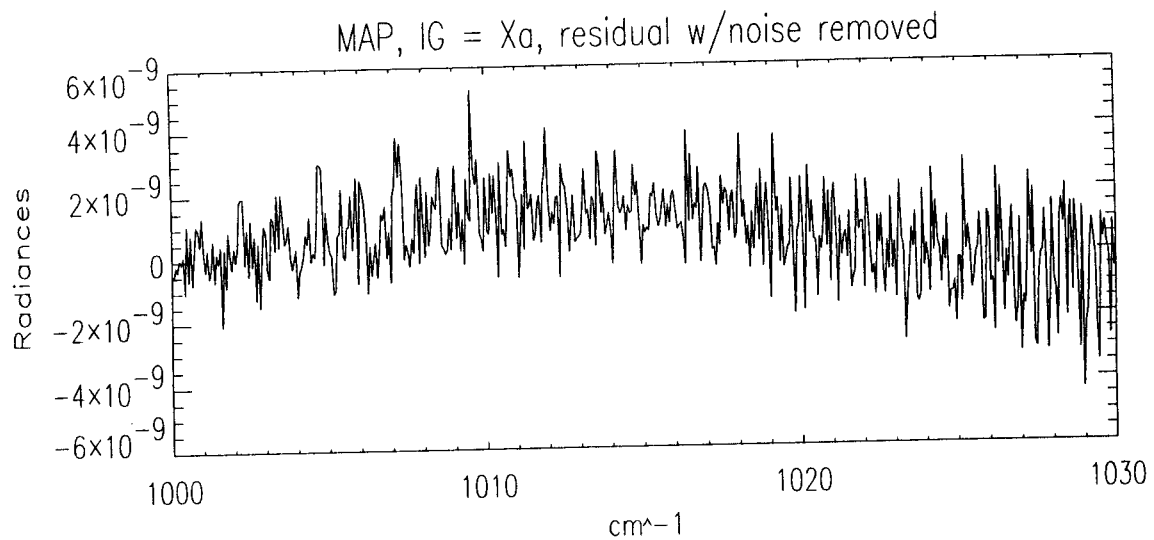
A priori covariance matrix



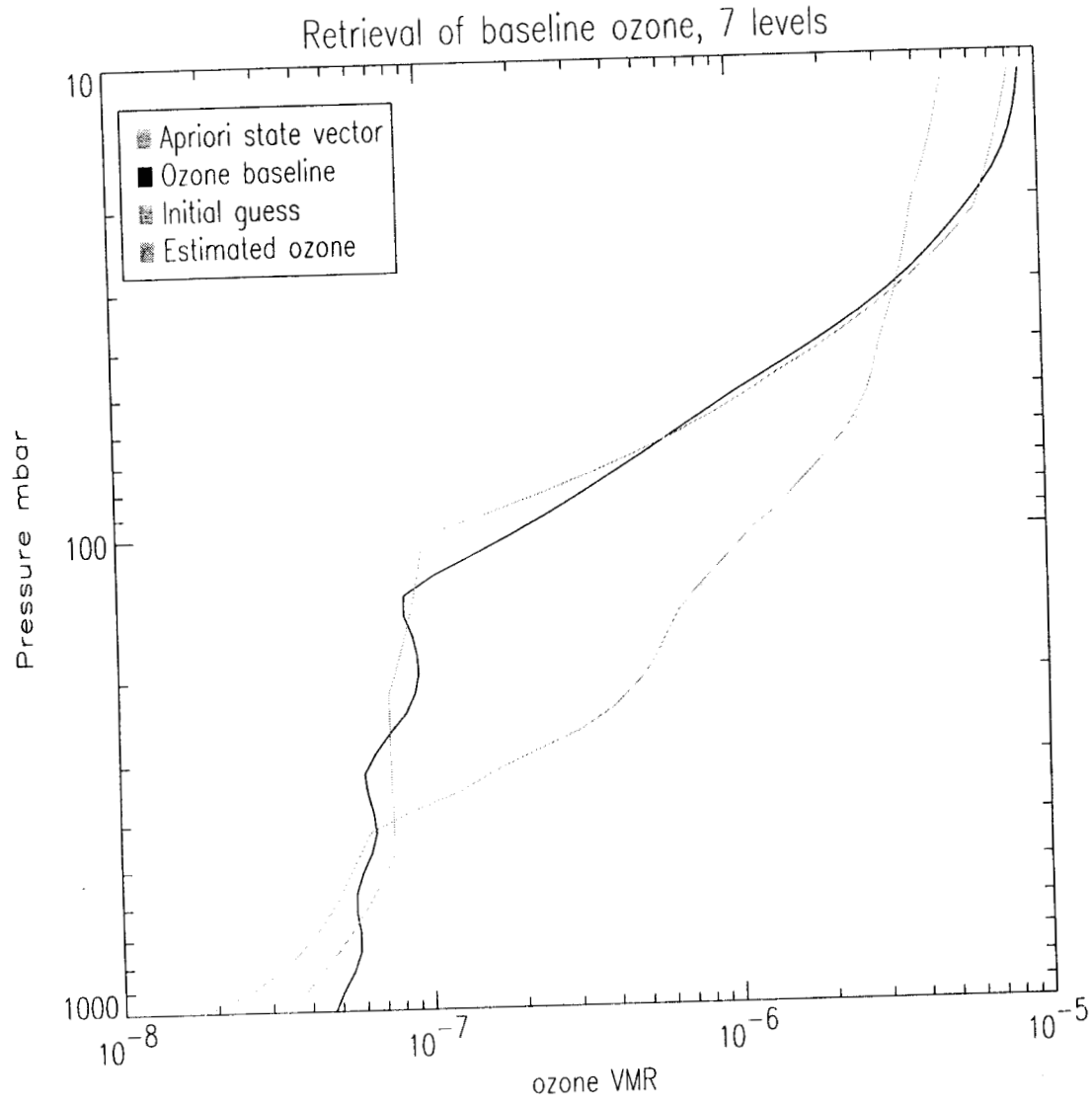
Retrieval of mid-latitude ozone

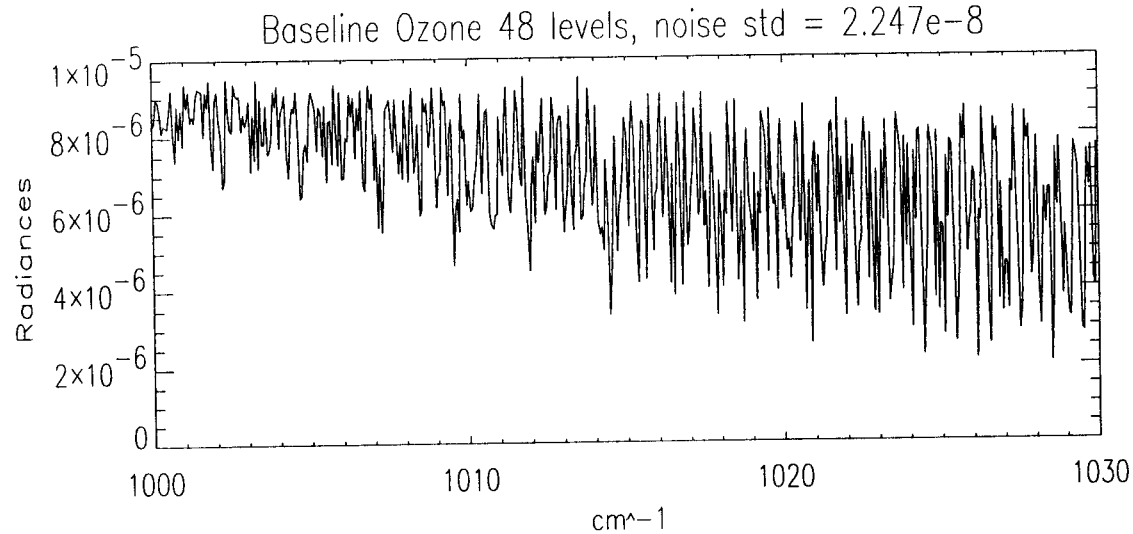


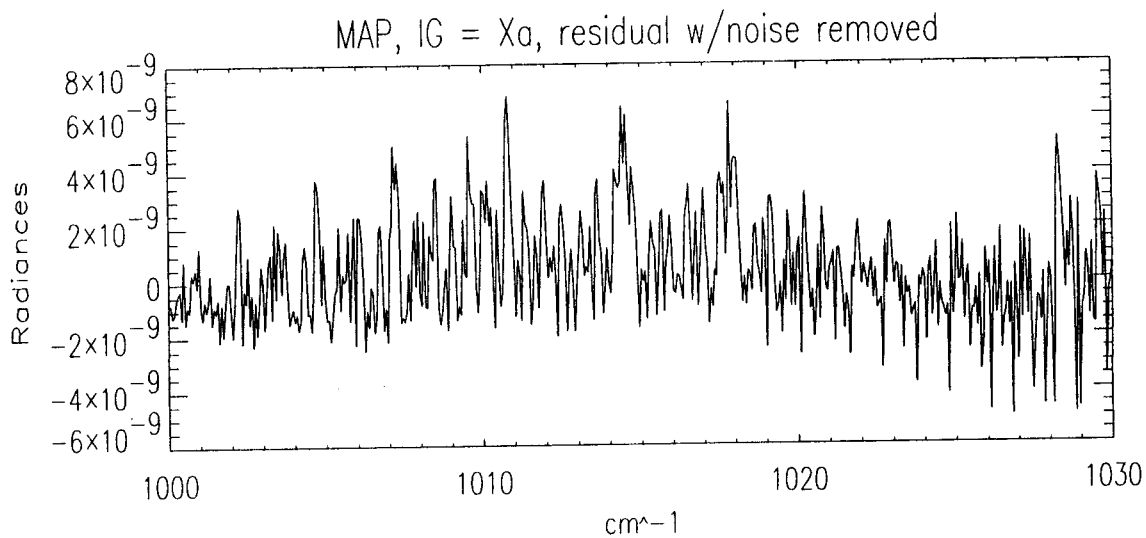

Baseline Ozone 48 levels, noise std = 2.247e-8
Radiances
1x10^-5
8x10^-6
6x10^-6
4x10^-6
2x10^-6
0
1000
1010
1020
1030
cm^-1


MAP, IG = Xa, residual w/noise removed
Radiances
6x10^-9
4x10^-9
2x10^-9
0
-2x10^-9
-4x10^-9
-6x10^-9
1000
1010
1020
1030
cm^-1

Retrieval of mid-latitude ozone with Alert station as initial guess




Baseline Ozone 48 levels, noise std = 2.247e-8
Radiances
1x10^-5
8x10^-6
6x10^-6
4x10^-6
2x10^-6
0
1000
1010
1020
1030
cm^-1


MAP, IG = Xa, residual w/noise removed
Radiances
8x10^-9
6x10^-9
4x10^-9
2x10^-9
0
-2x10^-9
-4x10^-9
-6x10^-9
1000
1010
1020
1030
cm^-1

Conclusions

- Optimal estimation provides the framework (ML,MAP) for atmospheric retrievals while optimization algorithms (GN,LM) provide the means of estimation.
- The trust region constrains the steps to be in an assumed linear region while the *a posteriori* measure adaptively updates this region.
- A simulated retrieval of mid-latitude ozone was performed using different a priori state vectors and initial guesses.
- The MAP-LM algorithm was able to successfully do a retrieval of mid-latitude ozone using a polar initial guess by using the respective strengths of the Levenberg-Marquardt algorithm and Bayesian framework.