united nations educational, scientific and cultural organization
international atomic energy agency

the
abdus salam
international centre for theoretical physics

Course on "Inverse Methods in Atmospheric Science"
1 - 12 October 2001

301/1332-1

"Optimal Spectral Inversion of Atmospheric Radiometric Measurements in the Near-UV to Near-IR Range: From Optical Thickness to Aerosol Size Distribution..."

Didier FUSSEN
Institut d'Aéronomie Spatiale de Belgique
Brussels, Belgium

Please note: These are preliminary notes intended for internal distribution only.

Optimal spectral inversion of atmospheric radiometric measurements in the near-UV to near-IR range: from optical thickness to aerosol size distribution...

Trieste, October 2001

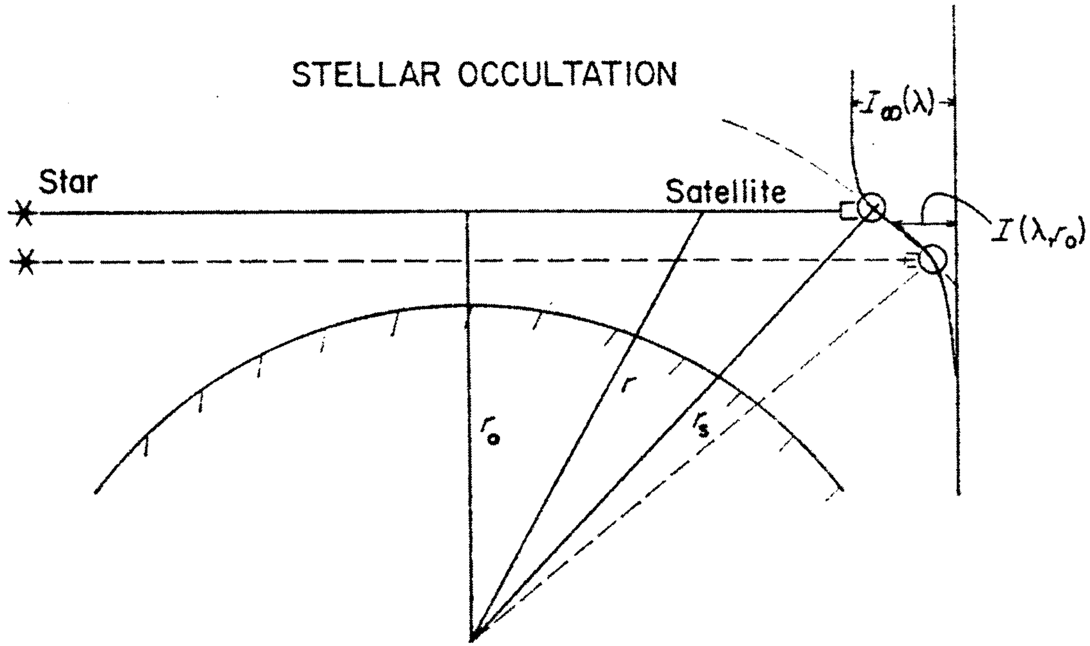
Didier FUSSEN

Institut d'Aéronomie Spatiale de Belgique

Contents

- Problems related to “spectral” inversion
- Problems related to “optical” inversion

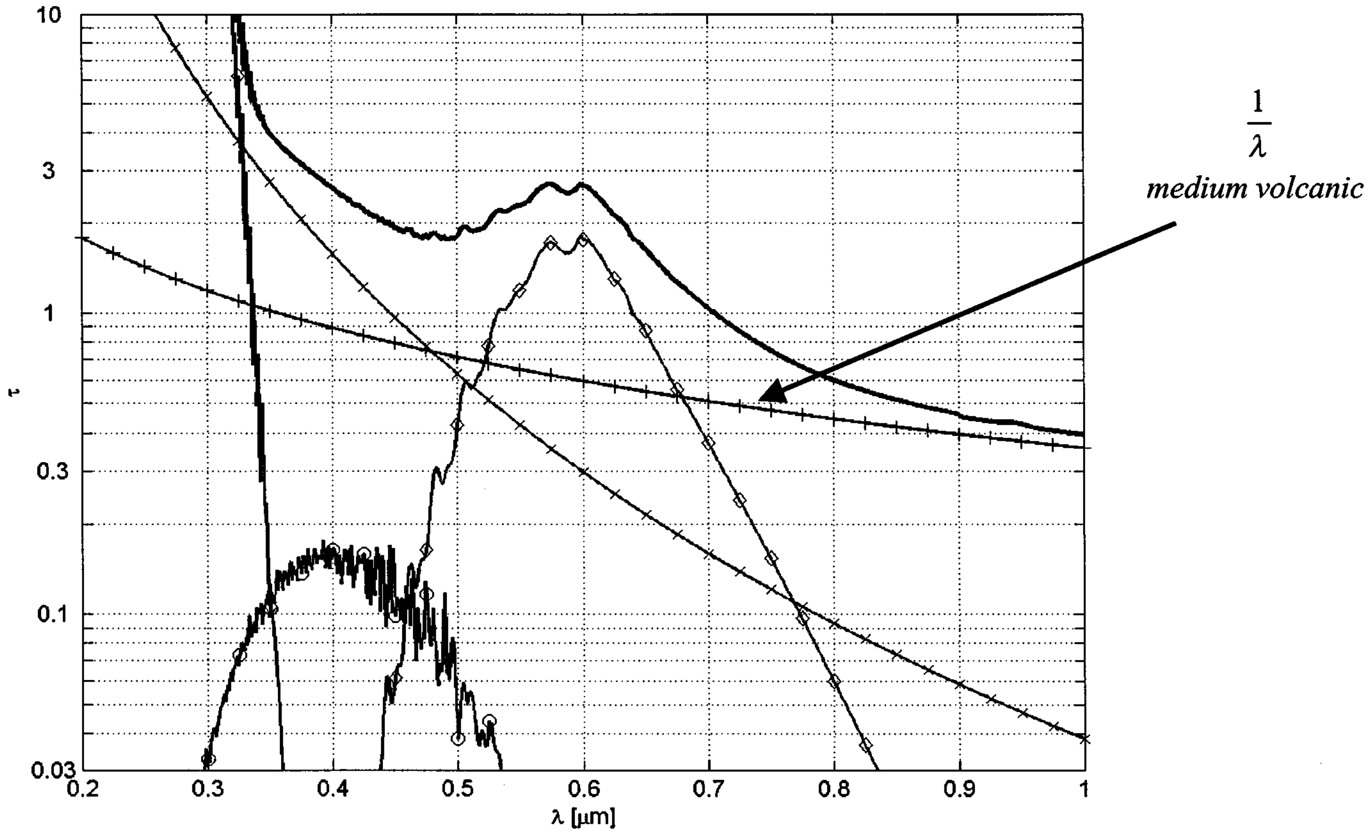
A simple occultation geometry...



$$T(r_0) = \frac{I(r_0)}{I_\infty} = e^{-\left(\bar{\tau}_{\mathrm{Air}\{N_2, O_2\}} + \tau_{O_3} + \tau_{NO_2} + \tau_{\mathrm{Aerosol}}\right)}$$

For most constituents: $\tau_i = \sigma_i n_i(s)ds \cong \sigma_i(cm^2)N(cm^{-2})$

For aerosols: $\tau_a = a_0 + a_1(\lambda - \lambda_0) + a_2(\lambda - \lambda_0)^2 + \ldots$



Performance of an infinite resolution spectrometer...

Measured : $\tau(\lambda)$

Modelled aerosol: use $\tau_n(\lambda) \propto (\lambda-\lambda_0)^n$

$$M(\lambda) = a_{N_2}\tau_{N_2}(\lambda) + a_{O_3}\tau_{O_3}(\lambda) + a_{N_2}\tau_{N_2}(\lambda) + \underbrace{a_0\tau_0(\lambda) + a_1\tau_1(\lambda) + \ldots a_n\tau_n(\lambda)}_{Polynomial\ \ aerosol}$$

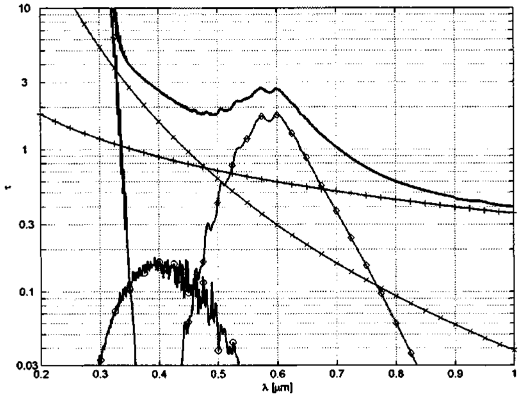
Merit function to be minimized

$$\chi = \int_{\lambda_1}^{\lambda_2} \left(\frac{\tau(\lambda) - M(\lambda)}{\delta\tau(\lambda)} \right)^2 d\lambda$$

$$\delta T = \sqrt{\frac{T}{S}}$$

We only consider shot noise.

Ex: S=10 000 => δT=0.01

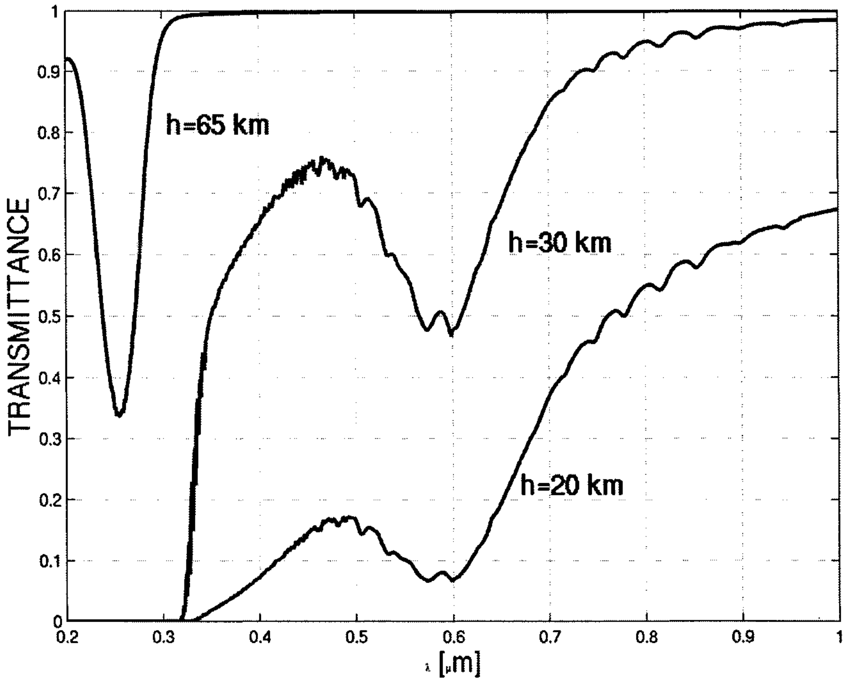


$$T = e^{-\tau} \quad ? \quad dT = -e^{-\tau} d\tau = -T d\tau$$

$$? \quad \delta\tau = \frac{1}{\sqrt{TS}}$$

$$\chi = \int_{\lambda_1}^{\lambda_2} \left(\frac{\tau(\lambda) - M(\lambda)}{\delta\tau(\lambda)} \right)^2 d\lambda$$

$$= \int_{\lambda_1}^{\lambda_2} \left(\tau(\lambda) - M(\lambda)\right)^2 S\,T(\lambda)\,d\lambda$$



Linear system: $C\vec{a}=\vec{b}$

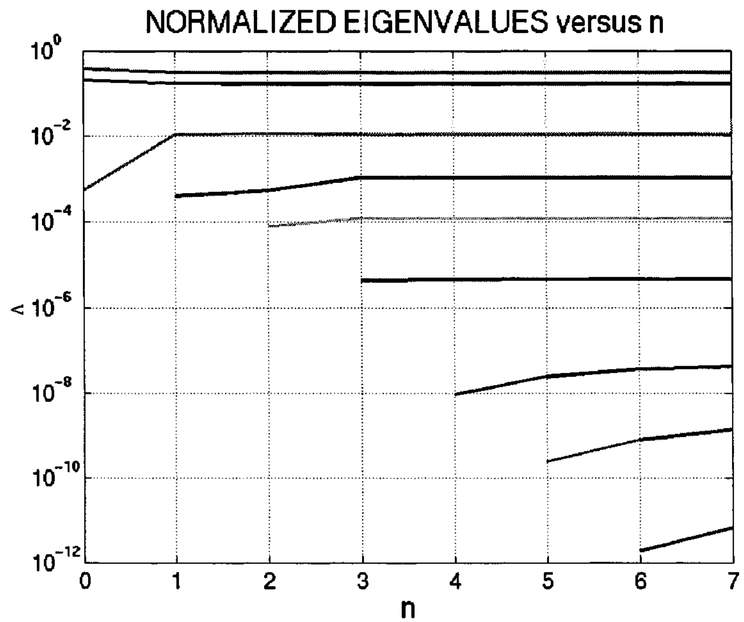
$$\langle \tau_i | \tau_j \rangle = \int_{\lambda_1}^{\lambda_2} \tau_i(\lambda)\tau_j(\lambda)\, S\, T(\lambda)\, d\lambda$$

$$
\left[\begin{array}{ccc:cccc}
\langle \tau_{N_2} | \tau_{N_2} \rangle & \langle \tau_{N_2} | \tau_{O_3} \rangle & \langle \tau_{N_2} | \tau_{NO_2} \rangle & \langle \tau_{N_2} | \tau_0 \rangle & \langle \tau_{N_2} | \tau_1 \rangle & \cdots & \langle \tau_{N_2} | \tau_n \rangle \\
\langle \tau_{N_2} | \tau_{O_3} \rangle & \langle \tau_{O_3} | \tau_{O_3} \rangle & \langle \tau_{O_3} | \tau_{NO_2} \rangle & \langle \tau_{O_3} | \tau_0 \rangle & \langle \tau_{O_3} | \tau_1 \rangle & \cdots & \langle \tau_{O_3} | \tau_n \rangle \\
\langle \tau_{N_2} | \tau_{NO_2} \rangle & \langle \tau_{O_3} | \tau_{NO_2} \rangle & \langle \tau_{NO_2} | \tau_{NO_2} \rangle & \langle \tau_{NO_2} | \tau_0 \rangle & \langle \tau_{NO_2} | \tau_1 \rangle & \cdots & \langle \tau_{NO_2} | \tau_n \rangle \\
\hdashline
\langle \tau_{N_2} | \tau_0 \rangle & \langle \tau_{O_3} | \tau_0 \rangle & \langle \tau_{NO_2} | \tau_0 \rangle & \langle \tau_0 | \tau_0 \rangle & \langle \tau_0 | \tau_1 \rangle & \cdots & \langle \tau_0 | \tau_n \rangle \\
\langle \tau_{N_2} | \tau_1 \rangle & \langle \tau_{O_3} | \tau_1 \rangle & \langle \tau_{NO_2} | \tau_1 \rangle & \langle \tau_0 | \tau_1 \rangle & \langle \tau_1 | \tau_1 \rangle & \cdots & \langle \tau_1 | \tau_n \rangle \\
\vdots & \vdots & \vdots & \vdots & \vdots & & \vdots \\
\langle \tau_{N_2} | \tau_n \rangle & \langle \tau_{O_3} | \tau_n \rangle & \langle \tau_{NO_2} | \tau_n \rangle & \langle \tau_0 | \tau_n \rangle & \langle \tau_1 | \tau_n \rangle & \cdots & \langle \tau_n | \tau_n \rangle
\end{array}\right]
\begin{bmatrix} a_{N_2} \\ a_{O_3} \\ a_{NO_2} \\ a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix}
=
\begin{bmatrix} \langle \tau | \tau_{N_2} \rangle \\ \langle \tau | \tau_{O_3} \rangle \\ \langle \tau | \tau_{NO_2} \rangle \\ \langle \tau | \tau_0 \rangle \\ \langle \tau | \tau_1 \rangle \\ \vdots \\ \langle \tau | \tau_n \rangle \end{bmatrix}
$$

C is real symmetric =>

$$C = U \Lambda U^T$$

$$C^{-1} = U \Lambda^{-1} U^T$$



- random error -> $C^{-1} = U\Lambda^{-1}U^T$ and $e_r^i = \sqrt{C_{ii}^{-1}}$

  - **Retrieved species are not spectrally orthogo** $\langle \tau_i | \tau_j \rangle = \int_{\lambda_1}^{\lambda_2} \tau_i(\lambda)\tau_j(\lambda)\, S\, T(\lambda)\, d\lambda \; ?\; 0$

    => cross-correlations

  - **Example: A 1/_⁴ aerosol is not optically distinguishable from Rayleigh scattering !**

    => an eigenvalue vanishes and C is singular

  - **For a large number of repeated measurements, mean random error = 0**

    $Note: for\ aerosol\ e_r(\lambda) = \sqrt{(\tau_0 \ldots \tau_n(\lambda))C^{-1}(\tau_0 \ldots \tau_n(\lambda))^T}$

    $Note: for\ aerosol\quad \varepsilon = \sqrt{\frac{\int_{\lambda_1}^{\lambda_2} e(\lambda)^2\, d\lambda}{\lambda_2 - \lambda_1}}$

- bias (systematic error)

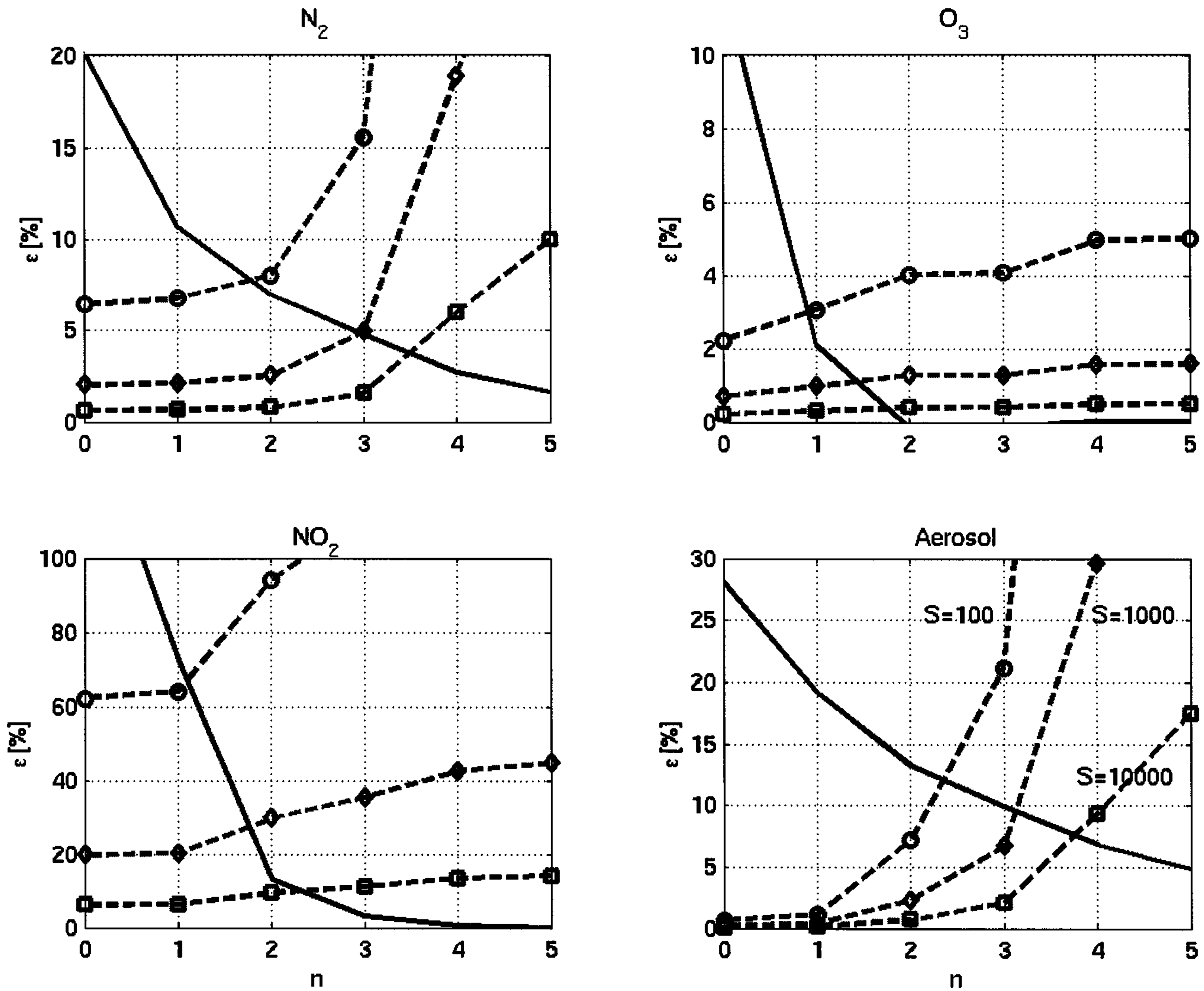
$$\Delta\tau_a(\lambda) = \tau_a^{\text{Exact}}(\lambda) - \sum_{i=0}^{n} a_i \tau_i(\lambda) \quad =>$$

$$\overrightarrow{\delta b} = <\Delta\tau_a(\lambda) \,|\, \overrightarrow{\tau_x(\lambda)}> \quad x = N_2, O_3, NO_2, 0, 1, \ldots n$$

$$\text{and} \quad \overrightarrow{e_b} = C^{-1}\overrightarrow{\delta b}$$

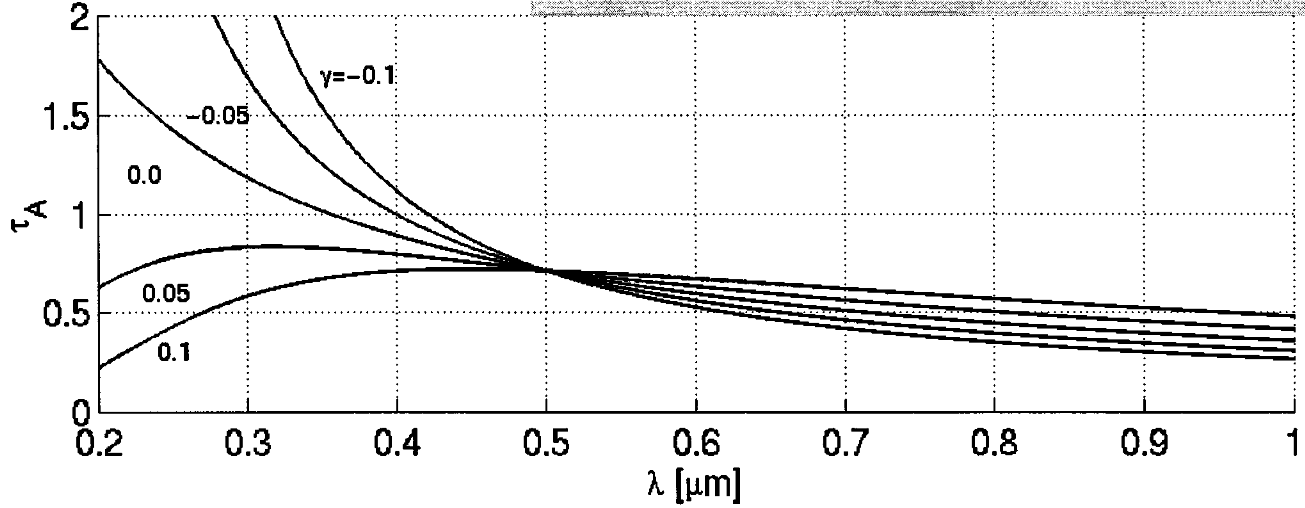
  - **"missing" aerosol information projects onto other species**
  - **bias error has a sign**
  - **bias error is also amplified by the inverse of covariance matrix**

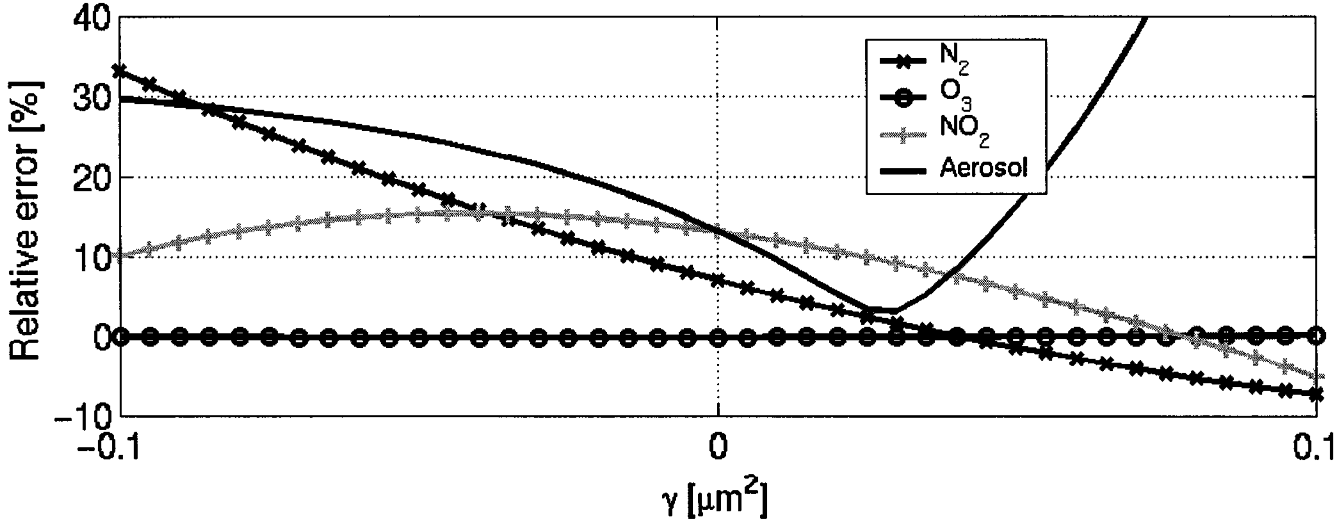
Trade-off between random and bias errrors versus aerosol polynomial degree (1/_ case) for different instrument sensitivities



Influence of the "true aerosol" spectral dependence on the bias error

$$\tau_A(\lambda) \propto e^{-\ln\left(\frac{1}{\lambda}\right)\left(\frac{\gamma}{\lambda^2}\right)}$$





Looking for alternative solutions…

- idea 1 : try to change the properties of the covariance matrix C

using full wavelength range increases statistics but it may amplify non-orthogonality

Change $\langle \tau_i | \tau_j \rangle = \int_{\lambda_1}^{\lambda_2} \tau_i(\lambda)\tau_j(\lambda)\, S\, T(\lambda)\, d\lambda$ in

$$\langle \tau_i | \tau_j \rangle = \int_{\lambda_1}^{\lambda_2} \tau_i(\lambda)\tau_j(\lambda)\, S\, T(\lambda) F(\lambda)\, d\lambda$$

where $F(\lambda)$ is a window function, e.g. $F(\lambda) = e^{-\left(\frac{\lambda - c_1}{c_2}\right)^2}$

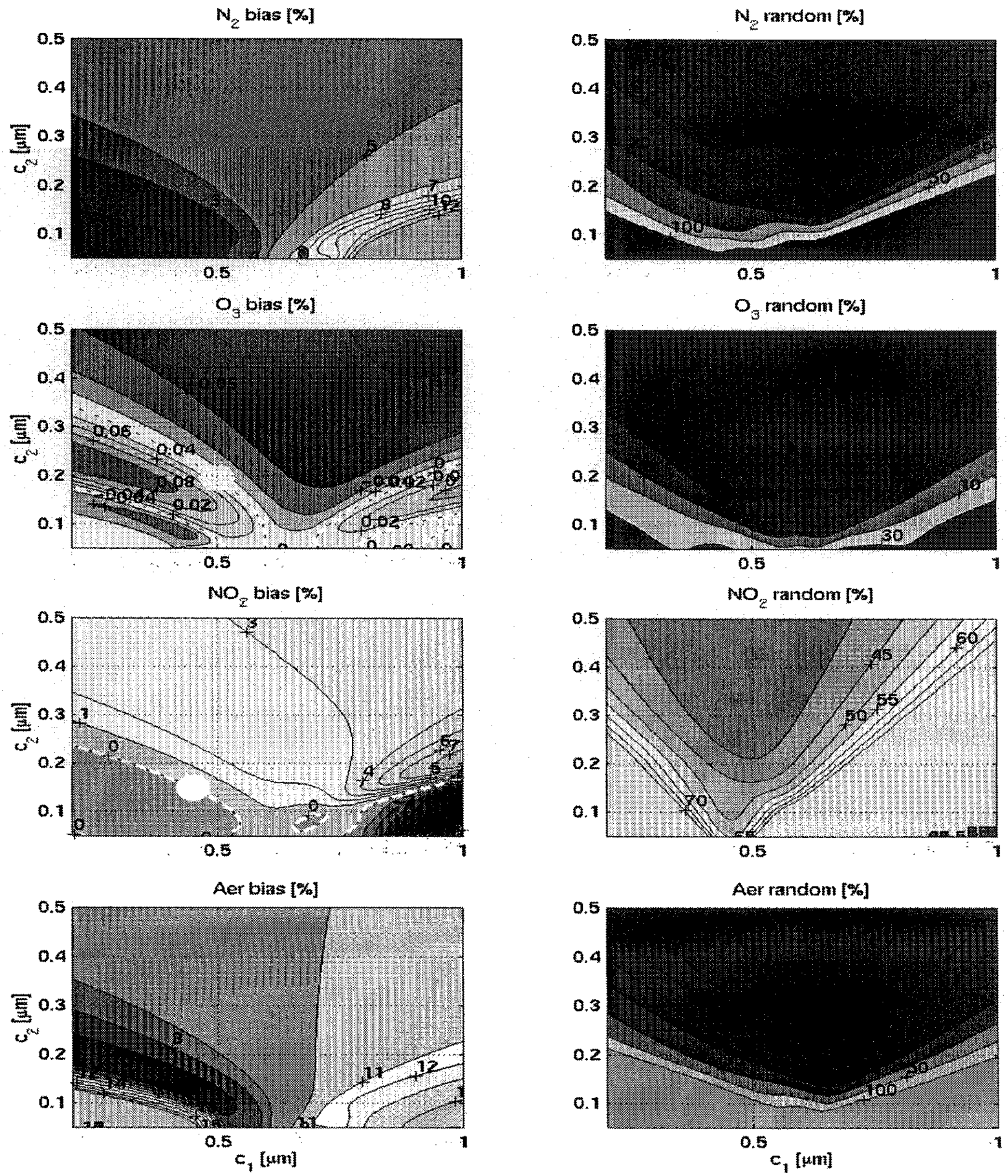
•Random error improves as c_2 increases. Bias error is not monotonic

• For N_2 , go to UV part and for aerosol stay in the visible, at expense of more random error. No clear benefit

•For O_3 and NO_2, there exist zero bias error isolines !

•Example: NO_2 optimization : Along the zero bias error isoline, minimize the random error.

	No window	Optimal window [c_1=0.45 c_2=0.148]
e_b [%]	12.5	0
e_r [%]	30.2	49.2
$(e_b^2+e_r^2)$	32.7	49.2



• <u>idea 2 : try to increases n while controlling the "smoothness" of the solution</u>

A classical regularization problem !

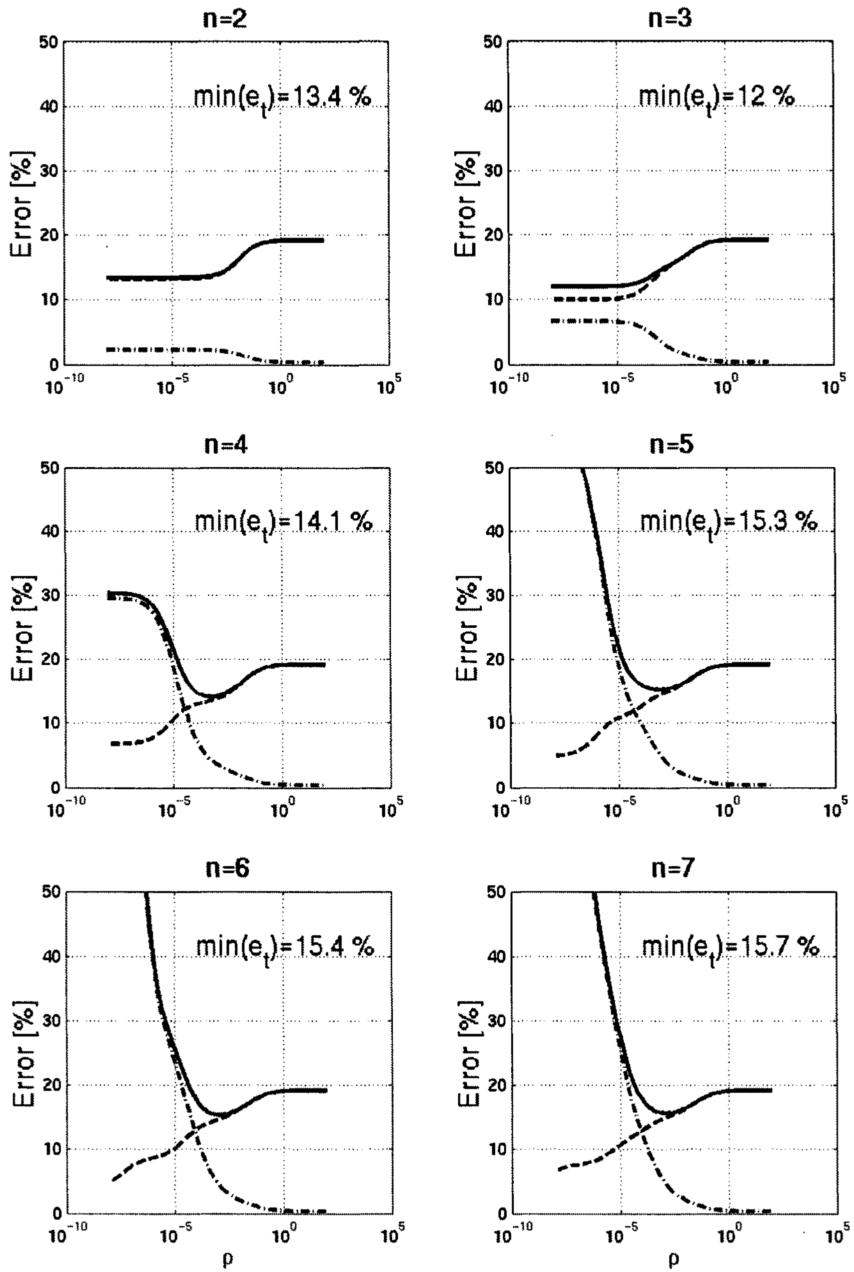
Objective: to fit measured data and to minimize global curvature of aerosol optical thickness $\tau_A(\lambda)$ simultaneously. It is necessary to define a new merit function:

$$\chi = \int_{\lambda_1}^{\lambda_2} \left(\frac{\tau(\lambda) - M(\lambda)}{\delta\tau(\lambda)} \right)^2 d\lambda + \rho \int_{\lambda_1}^{\lambda_2} \left(\frac{d^2\tau_A(\lambda)}{d\lambda^2} \right)^2 d\lambda$$

Closeness to data

Smoothness

- For **one** retrieval, we consider the behavior of e_b, e_r and total error $e_t=\sqrt{(e_b^2+e_r^2)}$ when the regularization parameter **r** is varied
- No miracle !



- <u>idea 3 : try to use large and small scale information</u>

Toward the DOAS method ...

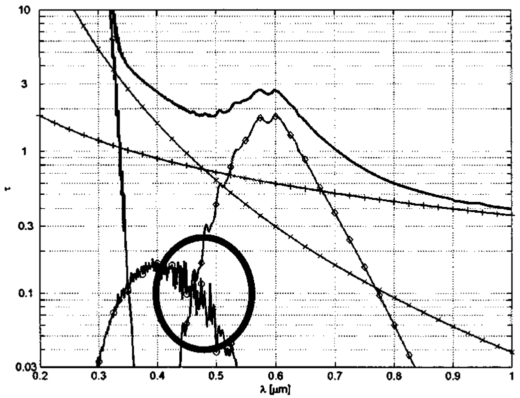
Objective: to fit measured data and first derivative of data simultaneously. Here again, we define an hybrid merit function:

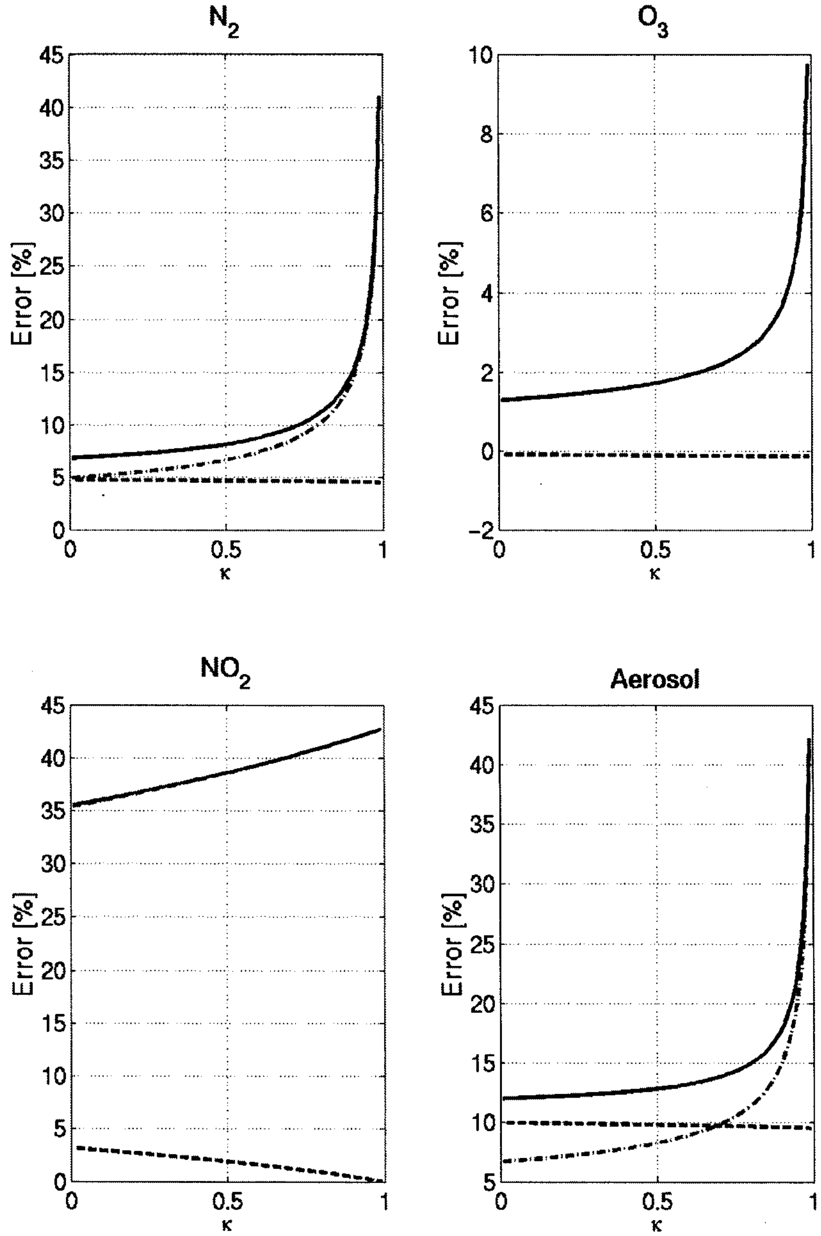
$$\chi = (1-\kappa)\int_{\lambda_1}^{\lambda_2}\left[\frac{\tau(\lambda)-M(\lambda)}{\delta\tau(\lambda)}\right]^2 d\lambda + \kappa\int_{\lambda_1}^{\lambda_2}\left[\frac{\tau'(\lambda)-M'(\lambda)}{\delta\tau'(\lambda)}\right]^2 d\lambda$$

Closeness to data

Closeness to data derivative

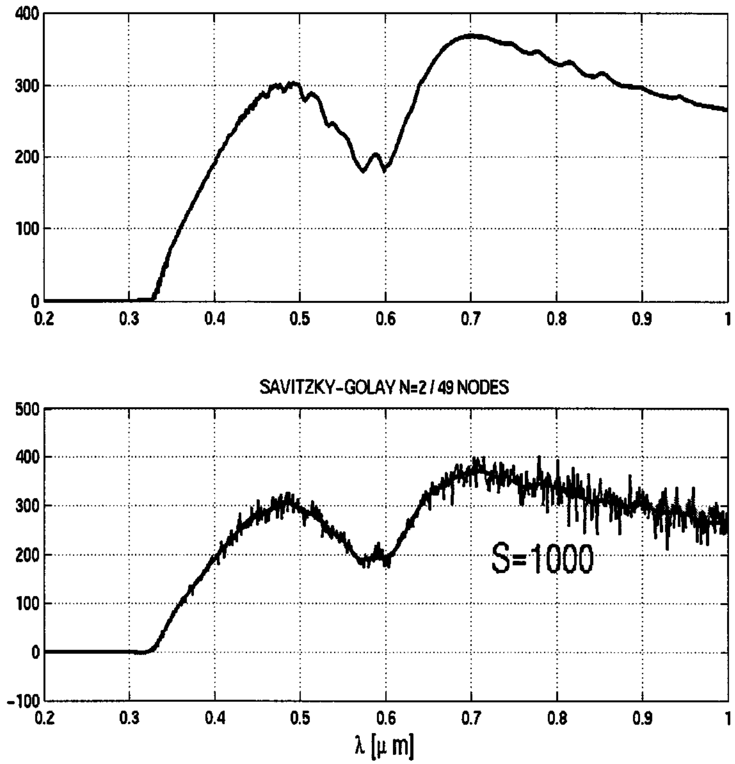
If the retrieved species does not exhibit sharp spectral features (like NO_2), the use of differential information is limited by higher noise sensitivity.





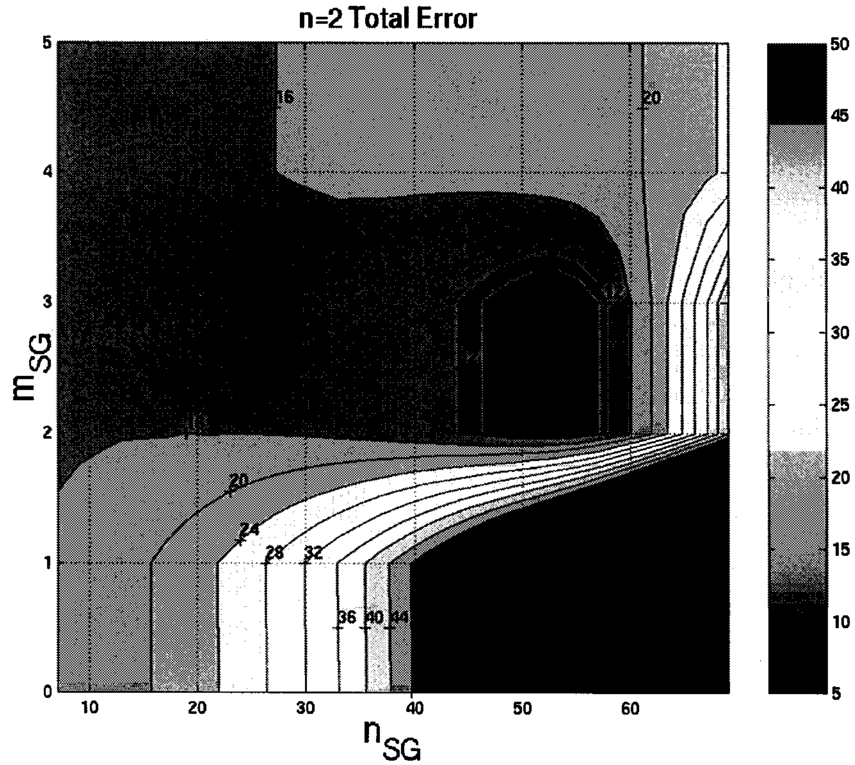
- idea 4 : use of filtering techniques

Objective: to get rid of high frequency noise which is overamplified by inversion. Only for low frequency species like aerosols.



Savitzky-Golay (sliding LS polynomial of order m_{SG} over n_{SG} nodes)

Gain is moderate but not negligible (Total error decreases from 14.4 % to 8.9 %)



Optical inversion

- **Information content is limited**
  - in UV-visible-nearIR: light diffracts on aerosol particle
  - in IR domain: light is absorbed by bulk aerosol

$$\beta(\lambda) = c_0 + c_1(\lambda - \lambda_0) + c_2(\lambda - \lambda_0)^2$$

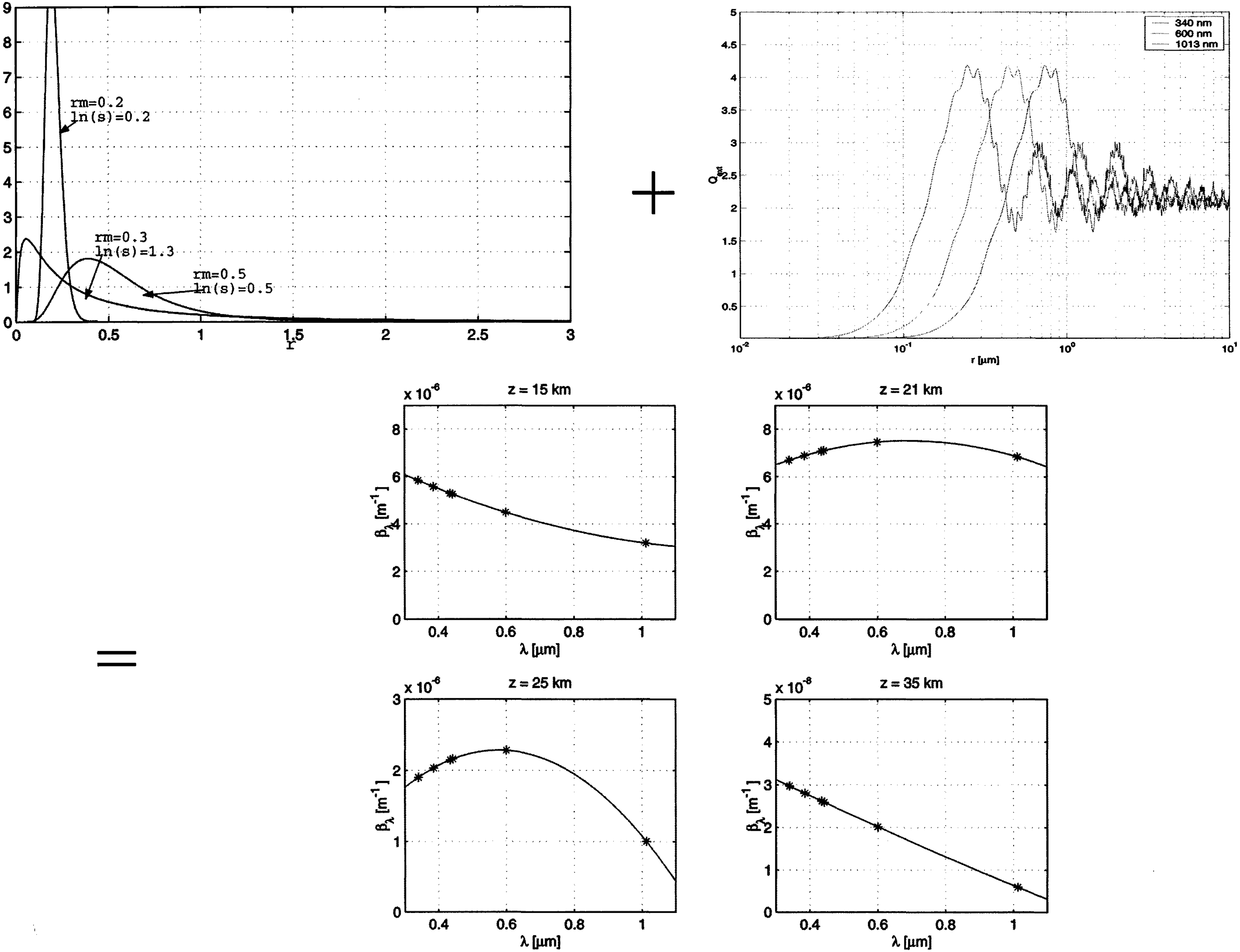
$$\beta_c(\lambda) = \int_0^{\infty} F(r)\, Q(r,\lambda)\, dr$$

$$F(r) = N \frac{1}{\sqrt{2\pi}\,\ln(\sigma) r} \exp\left(-\frac{\ln^2(r/r_m)}{2\ln^2(\sigma)}\right)$$

$\{c_0, c_1, c_2\}$

↓

$\{N, r_m, \ln(\sigma)\}$


rm=0.2
ln(s)=0.2
rm=0.3
ln(s)=1.3
rm=0.5
ln(s)=0.5
r
340 nm
600 nm
1013 nm
Q_{ext}
r [µm]
z = 15 km
z = 21 km
z = 25 km
z = 35 km
x 10^{-6}
x 10^{-6}
x 10^{-6}
x 10^{-8}
β_λ [m^{-1}]
λ [µm]

$$\beta(\lambda) = {}_{0}^{\times} F(r)\, Q(r,\lambda)\, dr \qquad F(r) = N \frac{1}{\sqrt{2\pi}\,\ln(\sigma) r} \exp\left(-\frac{\ln^2 (r/r_m)}{2\ln^2(\sigma)}\right) ? ?$$

---

1) Normalize theoretical and measured extinction coefficients

$$B_T(\lambda) \ldots \frac{\beta(\lambda)}{\beta(\lambda_*)} = f(r_m,\sigma) \qquad \text{idem for } B_M(\lambda)$$

---

2) Construct a merit function Ψ, at EACH retrieved altitude

$$\Psi = {}_{\lambda_i} \left(\frac{B_T(\lambda) - B_M(\lambda)}{\delta B_M(\lambda)} \right)^2 = \Psi(r_m,\sigma)$$

---

3) Minimize Ψ with respect to r_m and σ

$$\frac{f\Psi}{fr_m} = 0 \qquad \frac{f\Psi}{f\sigma} = 0$$

Ill-conditioning of merit function

- **Consider merit function at 3 adjacent altitudes -> it needs regulari**

$$r_m(z) = r_{min} + (r_{max} - r_{min})e^{-P_r(z)}$$

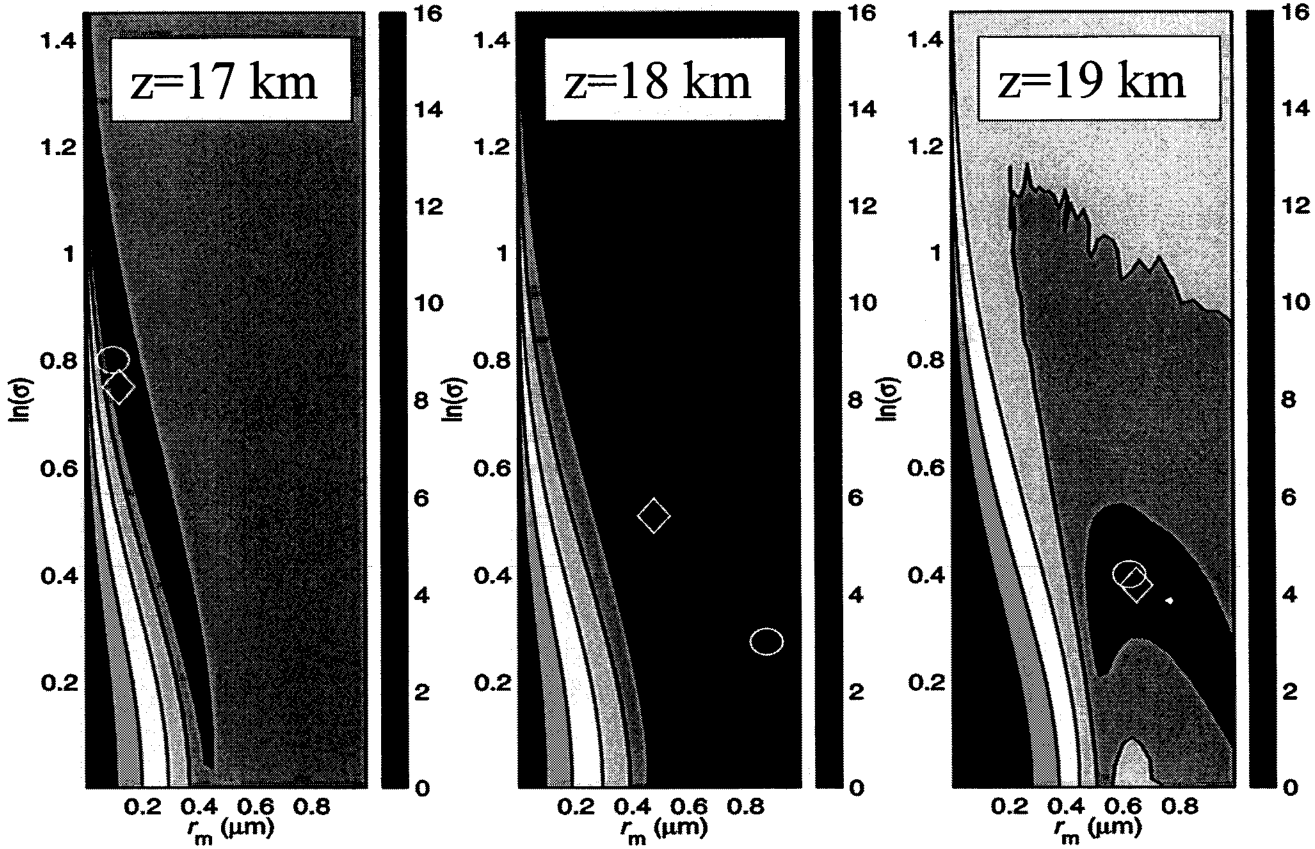
$$\sigma_m(z) = \sigma_{min} + (\sigma_{max} - \sigma_{min})e^{-P_\sigma(z)}$$

$$P_r(z) = \left(\mu_0 + \mu_1 z + \mu_2 z^2 + \ldots\right)^2$$

$$P_\sigma(z) = \left(\nu_0 + \nu_1 z + \nu_2 z^2 + \ldots\right)^2$$

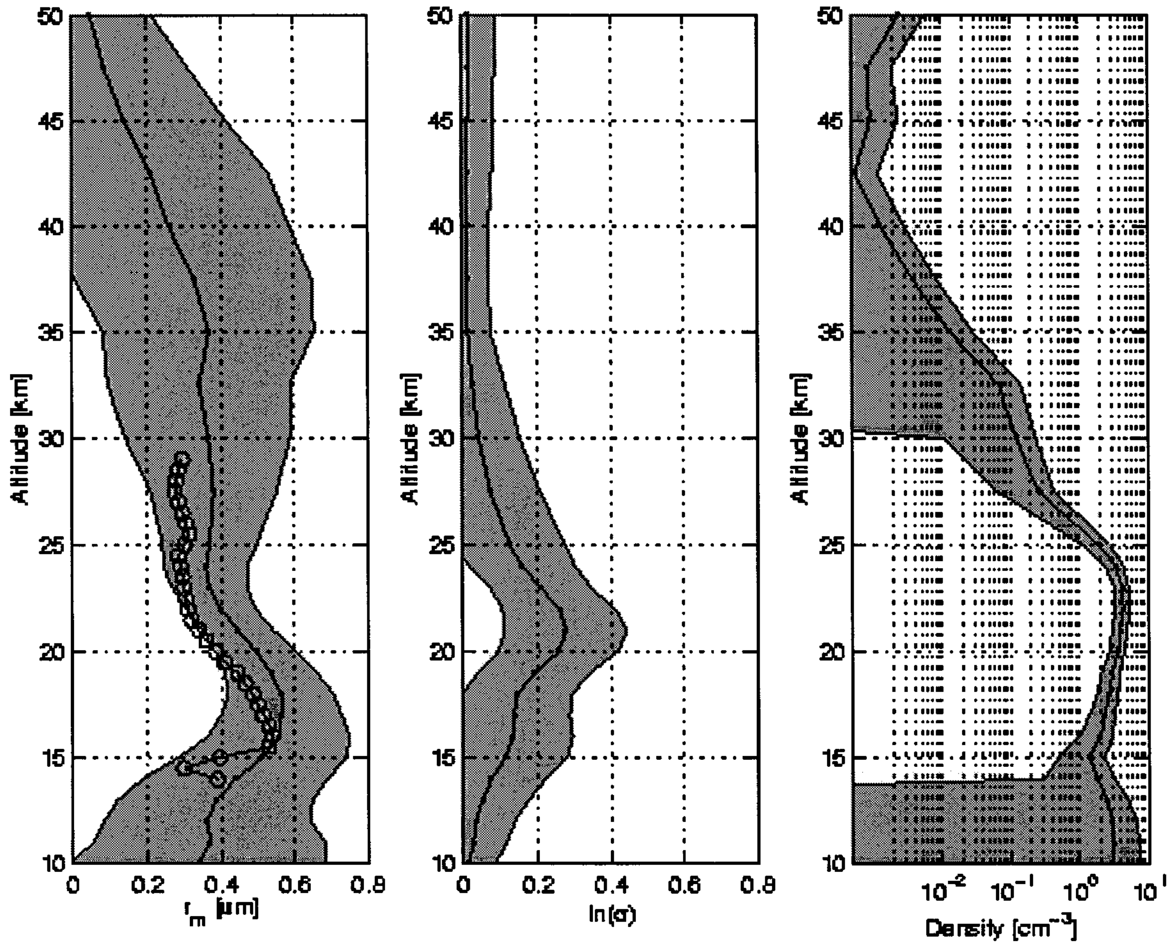
Optimize with respect to:

$$\{\mu_0, \mu_1, \mu_2, \ldots \nu_0, \nu_1, \nu_2, \ldots\}$$

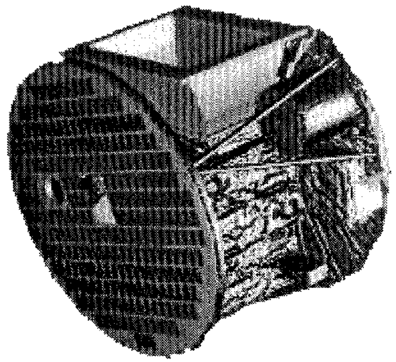


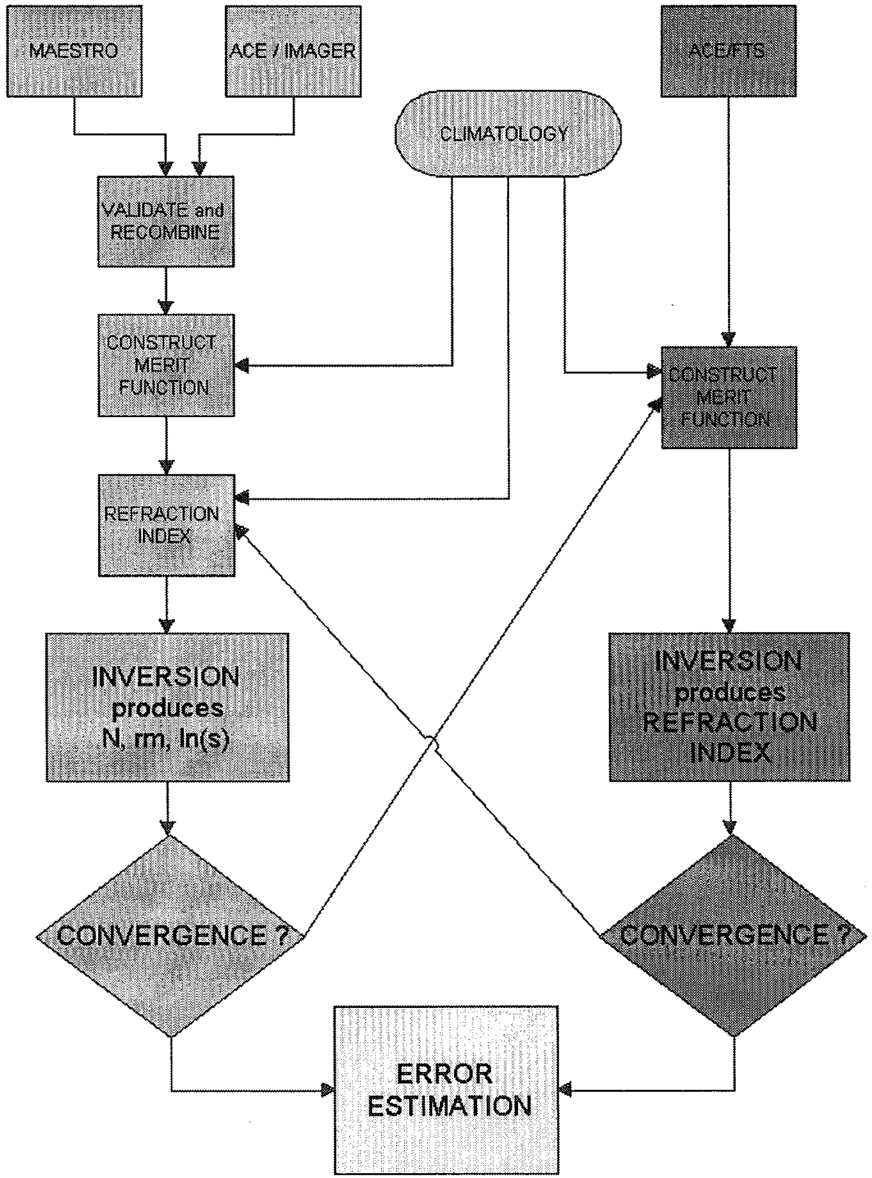
Post-volcanic period Aug. 92– May 93 / latitude 40°S–40°N

Mean profiles for r_m, $\ln(\sigma)$ and N



ACE / MAESTRO (end 2002)





Simple conclusions...

- Global spectral inversion is not "optimal"
- Optimal retrieval scheme can be constructed for particular species and objectives.
- Retrieval of aerosol size distributions can be improved by vertical regularization
- Open questions: order of inversions, filtering, use of auxiliary information,..