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ENVIAT Summer School 2003: Kyrölä: GOMOS retrieval

GOMOS

GOMOS retrieval

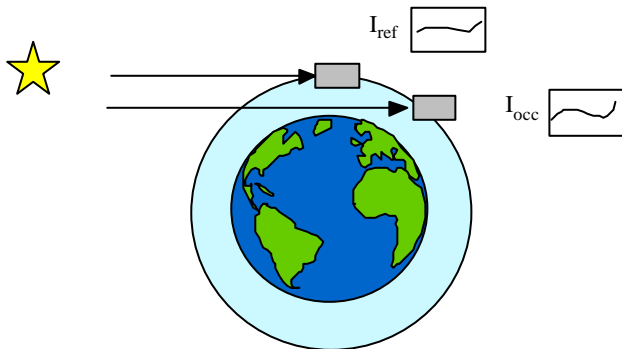
Erkki Kyrölä
Finnish Meteorological Institute

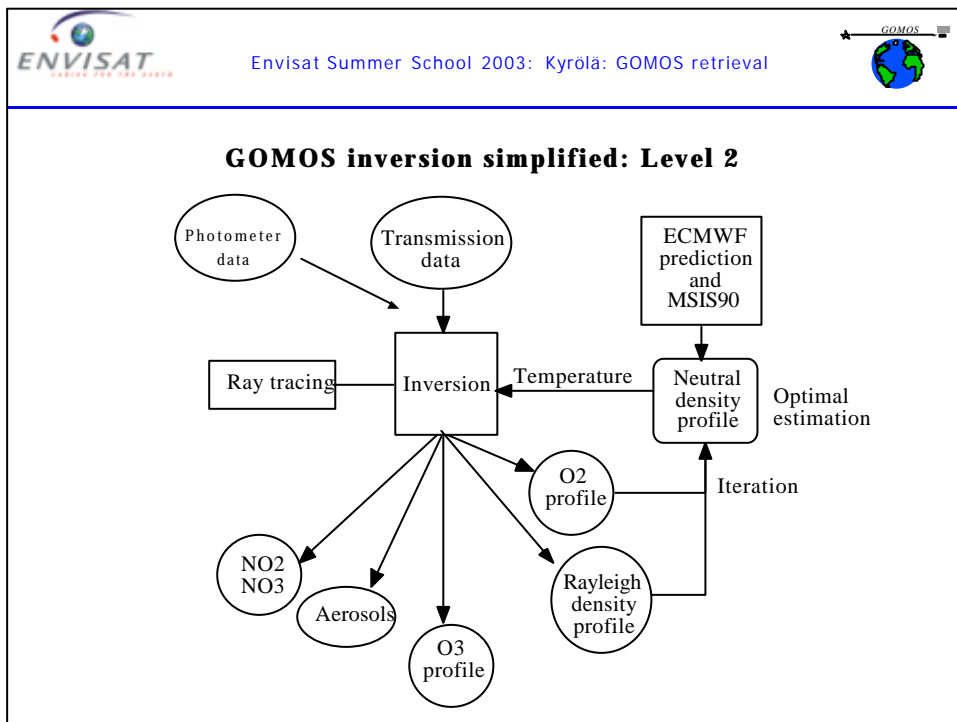
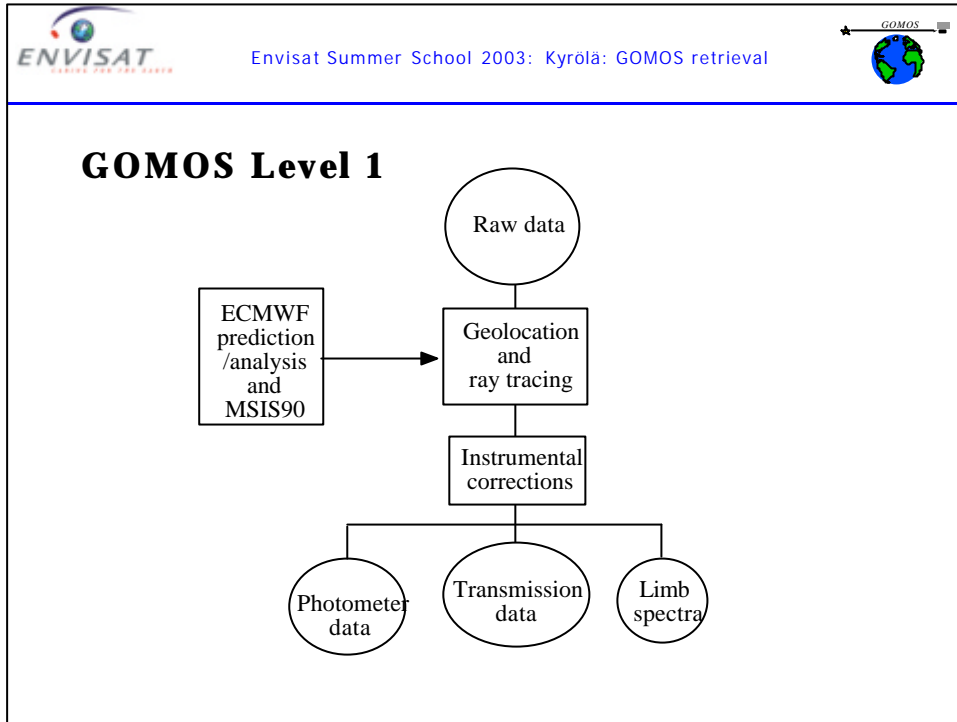
1. Overview
2. Spectral inversion
3. Vertical inversion
4. Validation
5. Advanced methods

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GOMOS

Global Ozone Monitoring by Occultations of Stars


$$T(\lambda) = \frac{I_{occ}(\lambda)}{I_{ref}(\lambda)}$$



When we were young

$$\frac{I_{\text{meas}}(z, \lambda)}{I_{\text{star}}(\lambda)} = T(\lambda) = e^{-\sigma(\lambda)N(z)}$$

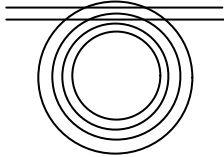
Beer's law

$$N(z) = -\frac{\log(T)}{\sigma(\lambda)}$$

$$N(z) = \int \rho(z(s)) ds$$

$$N = G \bar{\rho}$$


$$\bar{\rho} = G^{-1} N$$




Onion peeling

Level 2 inversion strategy

1. Single occultation at a time - no tomography
2. UVIS and IR transmissions are treated separately
3. Refractive dilution and scintillations effects are eliminated before the inversion using photometer and ray tracing data
4. Spectral and vertical inversions separated



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Transmission model for extinction

Transmission data to be compared
to the model transmission


$$T_{\text{mod}}(\lambda_k, t_j) = \int_0^L dW(\lambda - \lambda_k, t) e^{-\sum \sigma(\lambda, T(s)) \rho_j(s) ds}$$

where the LOS integration follows the refracted ray at wavelength λ .


Model simplifications:

1. Separate spectral and vertical inversions
2. Put the transmission model to the form:

$$T_{\text{mod}}(\lambda_k, t_j) = e^{-\tau}$$



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Separate spectral and vertical inversions

$$\tau = \sum \sigma_j(\lambda, T(s)) \rho_j(s) ds$$

$$= \sum \sigma_j^{\text{eff}}(\lambda) N_j \quad \text{separation of spectral and vertical problem}$$

$N_j = \int \rho_j(s) ds$ column density

$$\sigma_j^{\text{eff}}(\lambda) = \frac{\sum \sigma_j(\lambda, T(s)) \rho_j(s) ds}{N_j} \quad \text{effective cross section}$$

If a cross section is T-dependent, an iteration loop is needed

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**Spectral inversion:
uvis spectral inversion possibilities**

Linearization

Differential cross sections → $T_{\text{mod}} = e^{-\sum \sigma_j(\lambda) N_j}$

Spectral windows

Spectrally global (all data, no clean windows)

Absolute cross sections (aerosols, air)

Non-linear (noise is deformed by linearisation)

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Spectral inversion


We aim to minimize

$$S(N) = (T_{\text{obs}} - T_{\text{mod}}(N))^T C^{-1} (T_{\text{obs}} - T_{\text{mod}}(N))$$

C=covariance matrix
T=transmission vector (allt wavelengths)
N= column density vector (different constituents)

Solution by Levenberg-Marquard algorithm


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Residual = $T_{\text{model}} - T_{\text{observed}}$

Movie not included in this version

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Minimize


$$(T_{\text{mittaus}}(\mathbf{I}) - e^{-s_{\text{otsoni}}(\mathbf{I})N_{\text{otsoni}} - s_{\text{NO2}}(\mathbf{I})N_{\text{NO2}}})^2 \longrightarrow N_{\text{otsoni}} N_{\text{NO2}}$$

Interaction not included
 in this version


Movie not included
 in this version

Experiment
 (© P. Pirjola)

Levenberg-Marquardt
 (© J. Tamminen)



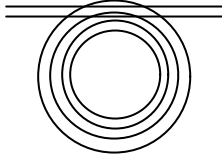
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Vertical inversion

$N = \int \rho(z(s)) ds$


Discretization of the atmosphere into layers:




$N = \sum \rho(s_i) \Delta s_i$

Simple matrix equation
 $N = \Delta \rho$

If number of layers=number of measurements,
 the onion peeling problem.



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Vertical inversion-profiles



In the GOMOS GS the densities are taken linear functions of altitude:

$$\rho(z) = \frac{(z_{j-1}-z)\rho_j + (z-z_j)\rho_{j-1}}{z_{j-1}-z_j}$$

This leads to a linear matrix equation

$$N = K \rho$$

which can be solved in standard methods.

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Iteration: level 2 loops

1. Effective cross section update:

After the first vertical inversion we can calculate the first real effective cross sections and carry out the spectral spectral and vertical inversion again.

2. New atmosphere:

After the vertical inversion we have obtained new estimates for neutral density and temperature. Thid data (if reliable) can be used in the calculation of the temperature dependent cross sections. We may also carry out a new ray tracing calculation.

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Iteration: Gomos atmosphere

1. In Level 1 the atmosphere (density and temperature) is formed from:

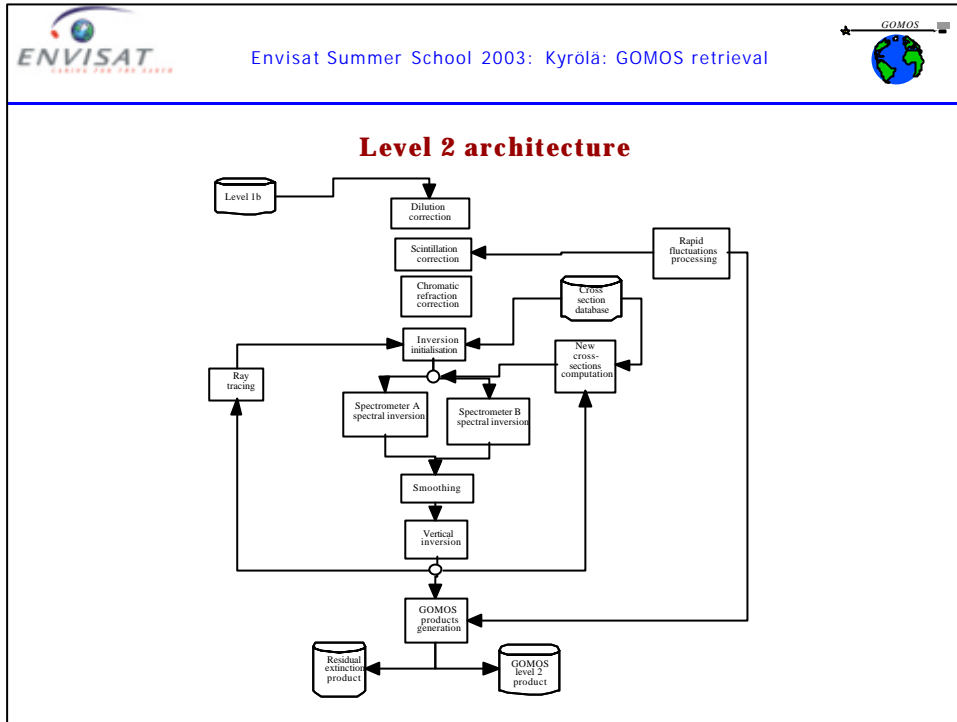
- A. ECMWF analysis or forecast
- B. MSIS90 model above ECMWF data

2. After one iteration over spectral-vertical inversion a new density and temperature profile can be derived from:

- A. Rayleigh extinction
- B. O2 absorption in IR spectrometer
- C. Time delay between the two photometers

Additional sources could be

- Refractive dilution
- O3 temperature dependent cross sections
- Star pointer angle i.e. refraction angle (Level 1)
- Rayleigh scattering in background term (not ESA product)



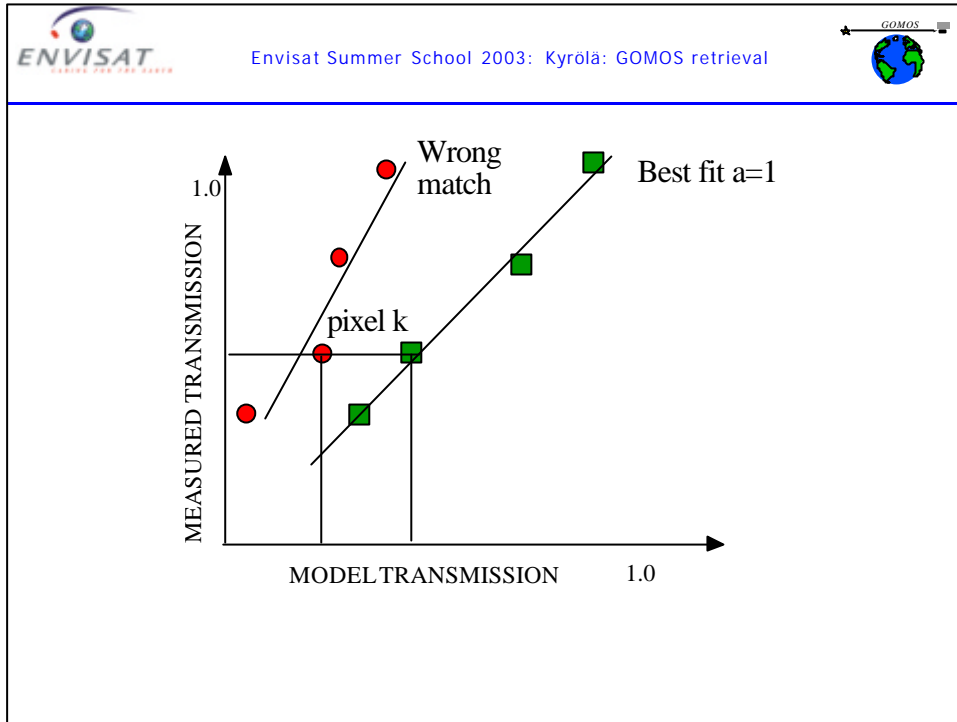
IR SPECTRAL INVERSION

The direct inversion used for the UVIS- spectrometer cannot be used for IR-spectrometer because the model transmission is computationally too demanding.

Therefore we use a method which compares the measured transmission and a series of pre-calculated model transmissions (each differing by the value of the column density of O₂ or H₂O):

$$T_{\text{obs}}(\lambda) \leftrightarrow T_{\text{mod}}(\lambda, N)$$

$$y = a \log(T_{\text{mod}}(\lambda, N)) + \frac{b}{\lambda} + c$$



High resolution temperature profile

By correlating the time series of blue and red photometers,
a time delay of the rays can be found.
From it we can derive the fine structured refraction angle.

$$\delta_{\text{blue}} - \delta_{\text{red}} = \frac{v_z \Delta t}{L} \quad \delta_{\text{blue}} = \frac{\delta_{\text{blue}} - \delta_{\text{red}}}{\Delta m/m}$$


From the refraction angle we can find the refractive index

$$m(h_{\text{blue}}) = \frac{1}{\pi} \frac{\delta_{\text{blue}}(h) dh}{\sqrt{(R+h)^2 - (R+h_{\text{blue}})^2}}$$


Finally the neutral density is given by

$$\rho(z) = \rho_s \frac{m(h_{\text{blue}}(z))}{a(\lambda)}$$

and the high resolution temperature can be calculated



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Consistency

1. In Level 1 the atmosphere (density and temperature) is formed from:
 - A. ECMWF analysis or forecast
 - B. MSIS90 model above ECMWF data


2. After one iteration over spectral-vertical inversion a new density and temperature profile can be derived from:
 - A. Rayleigh extinction
 - B. O₂ absorption in IR spectrometer
 - C. Time delay between the two photometers

Additional sources could be

- Refractive dilution
- O₃ temperature dependent cross sections
- Star pointer angle i.e. refraction angle (Level 1)
- Rayleigh scattering in background term (not ESA product)

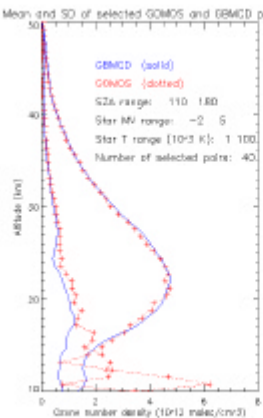


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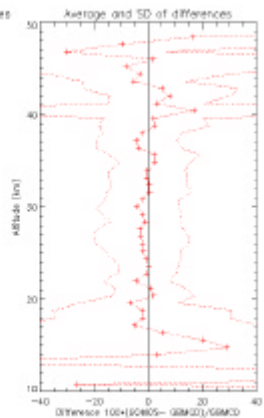


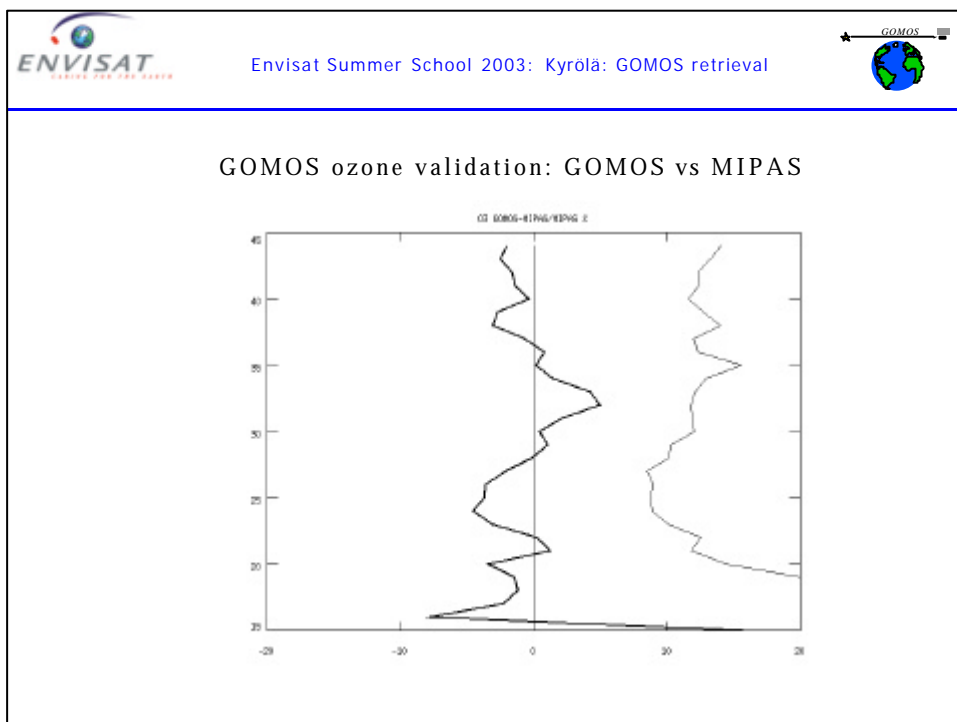
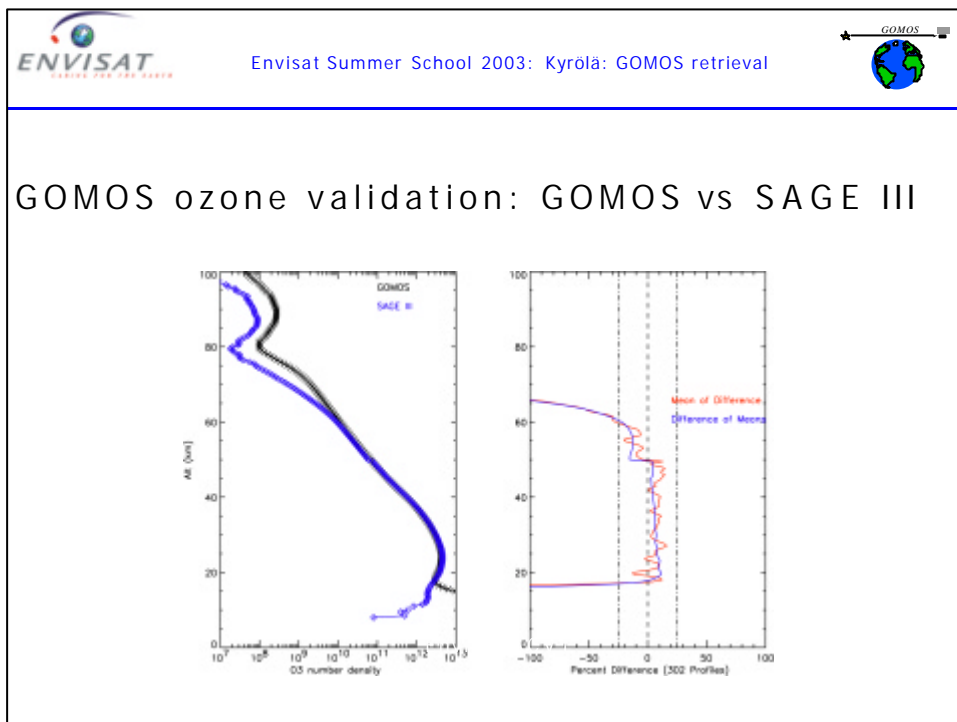
Statistical comparison for lidars (40 cases)

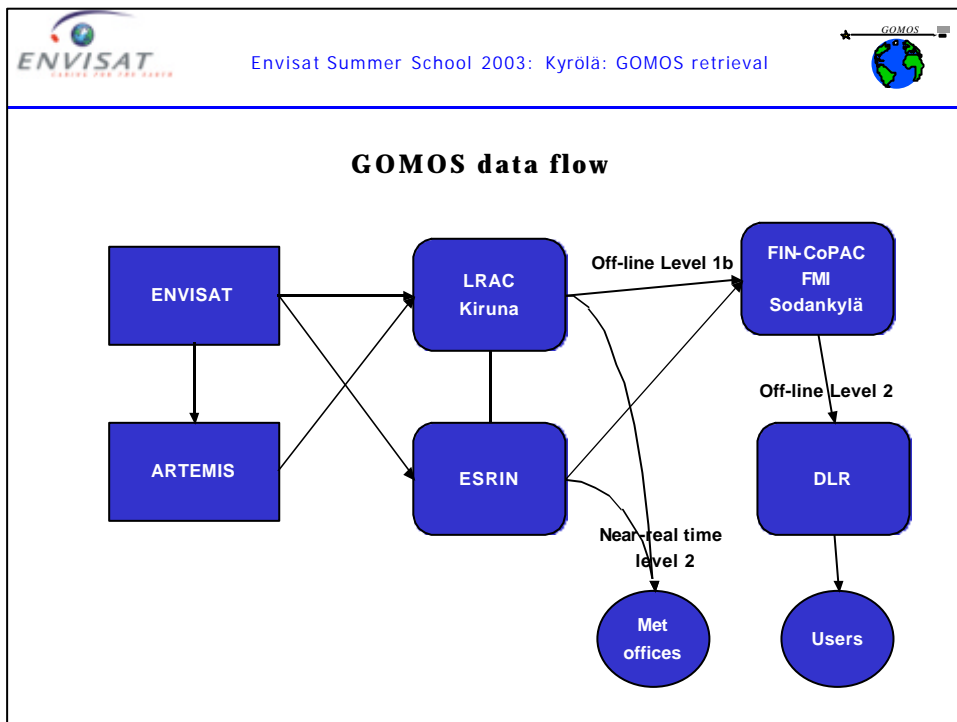
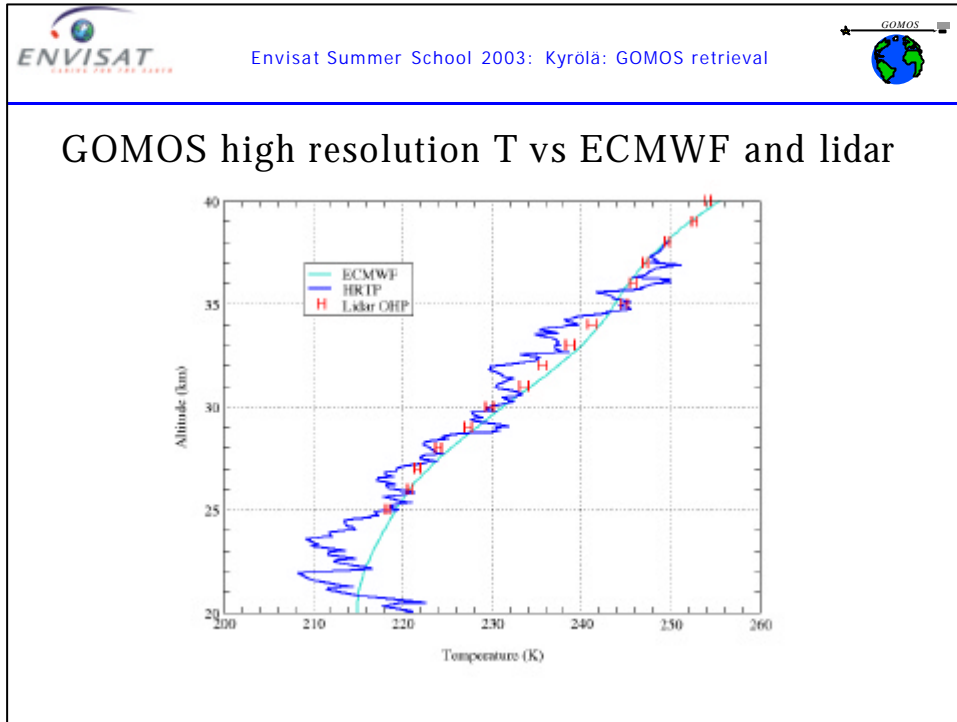
Mean and SD of selected GOMOS and GBMCD profiles



Average and SD of differences







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Future developments: one-step

```

    graph LR
      L1((Level 1 data)) --> SI[Spectral inversion]
      SI --> VI[Vertical inversion]
      VI --> L2((Level 2 data))
      L1 --> OSI[One-step inversion]
      OSI --> L2
      SI --> VI
  
```

No of wavelengths=1500 No of gases=5
 Number of layers=70 Number of layers=70
 i.e. 105000 data points i.e. 350 unknowns

But:
it works!

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Bayesian estimation


$$P(m|d) = \frac{P(d|m)P(m)}{P(d)}$$

where
 m=parameter(s) to be estimated
 d=data
 P(m)= a priori distribution of m
 P(d|m)= likelihood function
 P(m|d)= posteriori probability density of m

$$P(N|T_{obs}) = e^{-(T_{obs} - e^{-\sum N\sigma})^2} e^{-(N - N_{pr})^2}$$



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Posterior density

Posterior density $P(m|d)$ includes **all the information** we have on the measurements, modelling and prior information.

But how to make use of it? How to characterise the distribution and how to find estimators?

$\langle m \rangle = \int P(m|d) m \, dm$


$m_{pr} = \max(P(m|d))$

For **linear, Gaussian problems**, things are straightforward


$P(m|d) = e^{-\frac{1}{2}(m-\langle m \rangle)^T Q (m-\langle m \rangle)}$

For others:

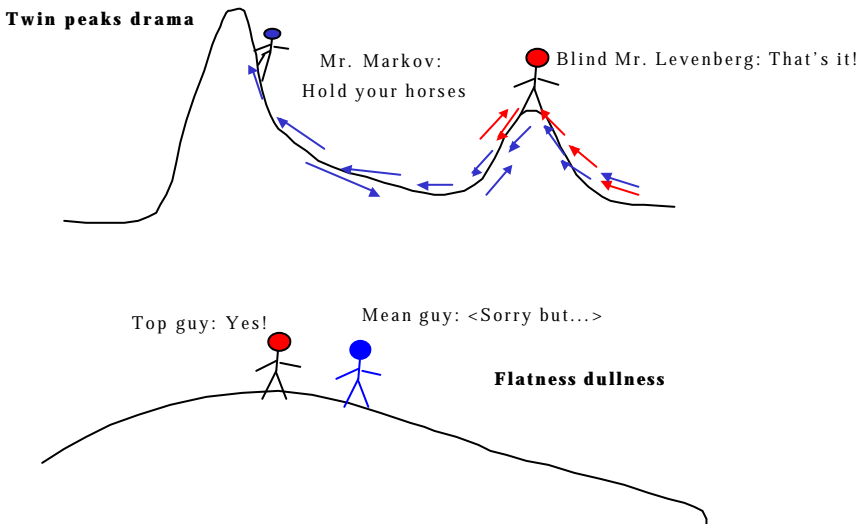
- are there multiple minima, flat regions, valleys, ridges?
- what are "good" estimators for complicated distributions?



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Ultimate estimators: Markov chain Monte Carlo



Twin peaks drama

Mr. Markov: Hold your horses

Blind Mr. Levenberg: That's it!

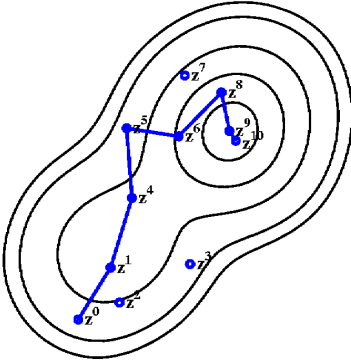
Top guy: Yes!

Mean guy: <Sorry but...>

Flatness dullness

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Markov chain Monte Carlo

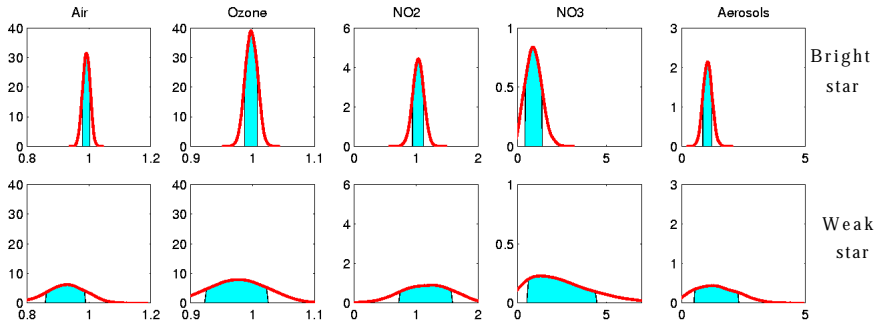


Estimators from MCMC

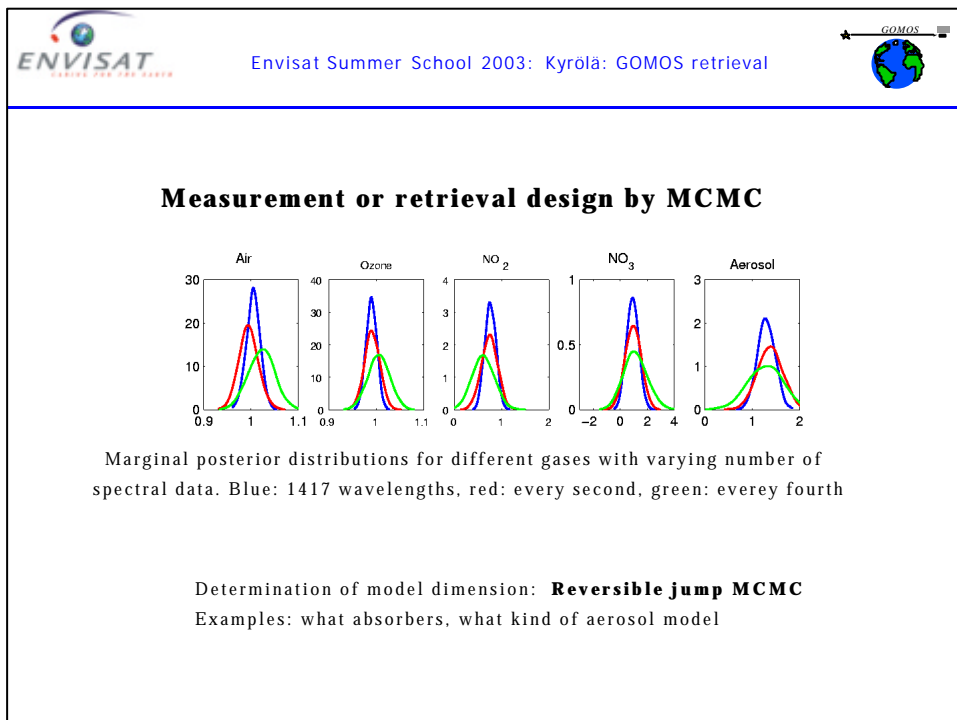
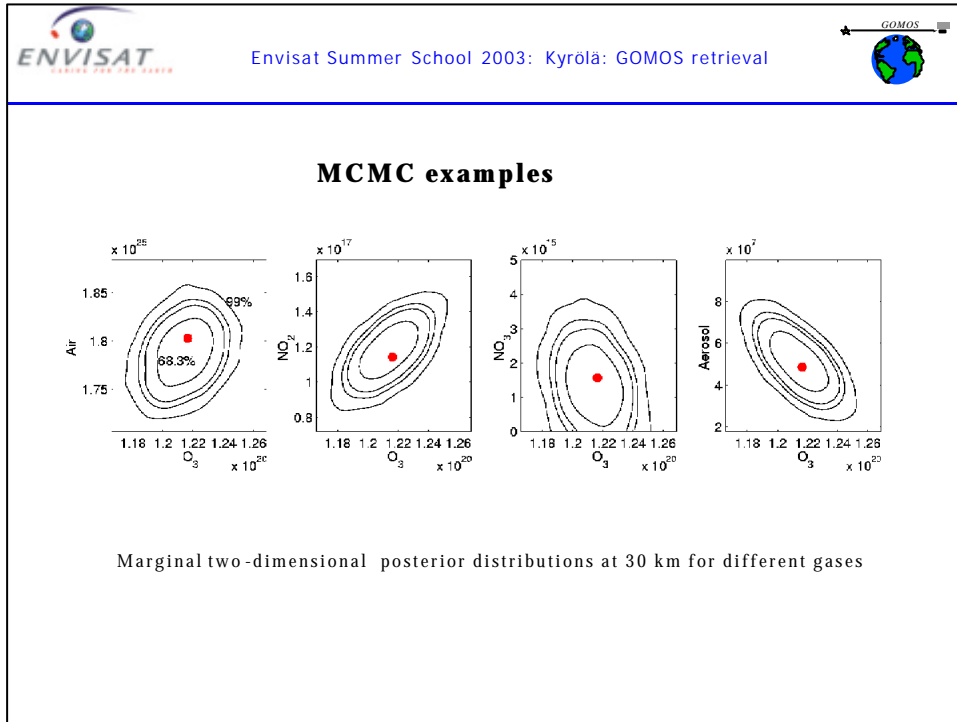
$$\langle X_i \rangle = \frac{1}{N} \sum_t^N Z_i^t$$

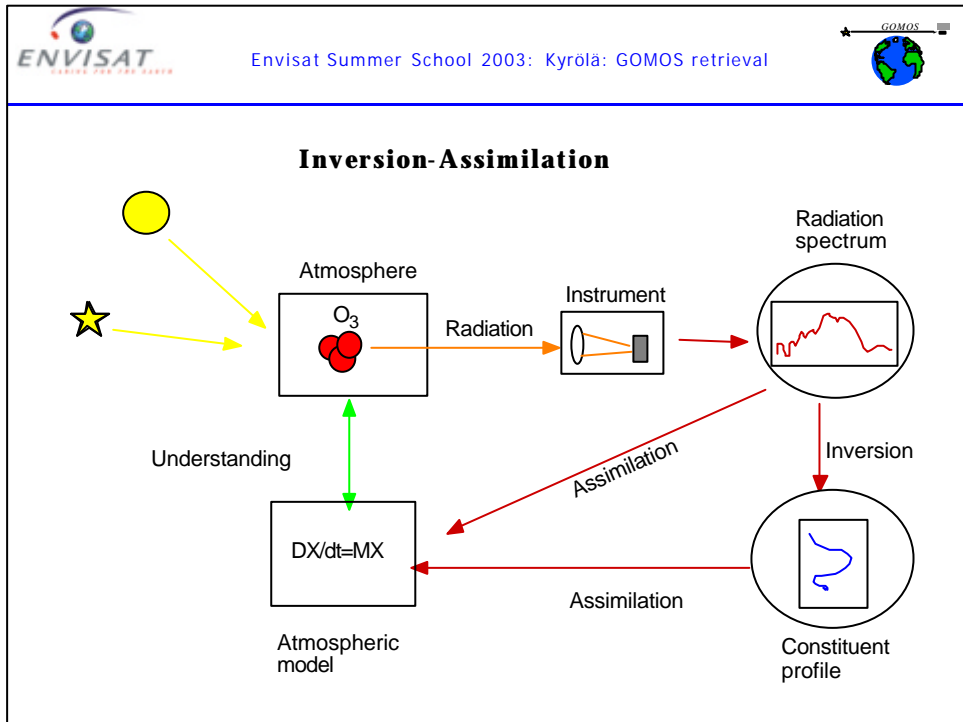
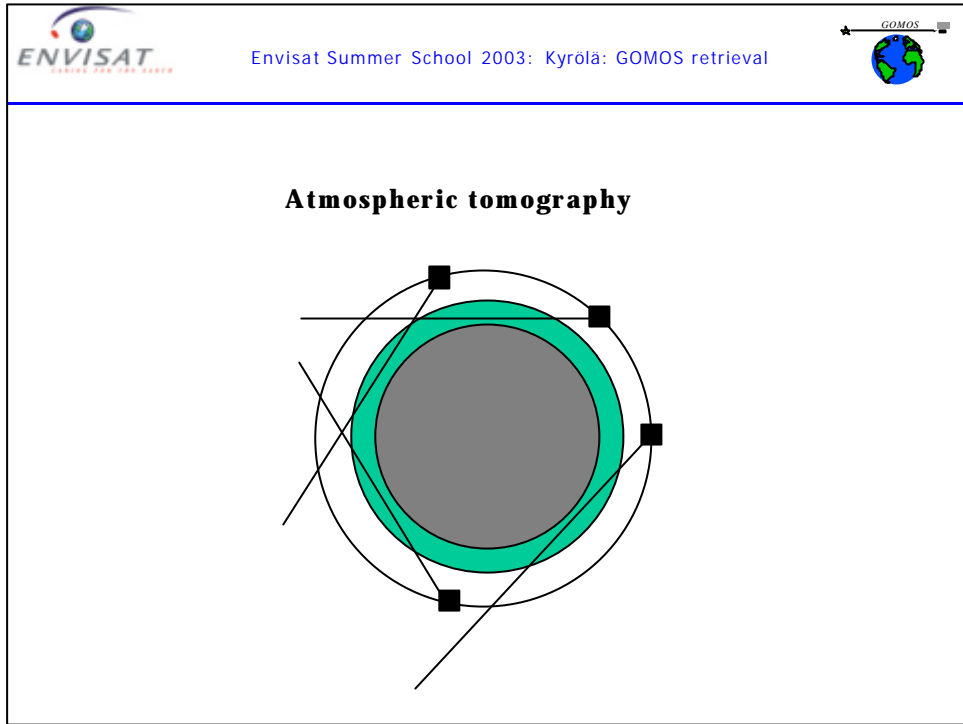
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MCMC examples



Marginal posterior distributions at 30 km for different gases





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More info

Inversion

Tarantola: Inverse problem theory, Methods for data fitting and model parameter estimation, Elsevier, 1987
Rodgers: Inverse Methods for Atmospheric Sounding : Theory and Practice, World Scientific, 2000

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Kyrölä et al, JGR, 98, 7367,1993 (Spectral inversion)
Tamminen and Kyrölä, JGR, 106, 14377, 2001 (MCMC)
ATBD-document: <http://envisat.esa.int/>