GOMOS retrieval

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

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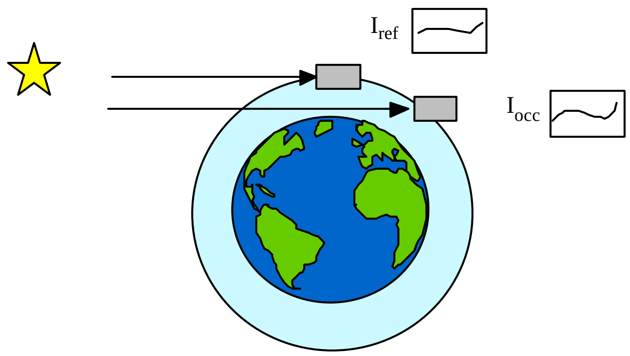
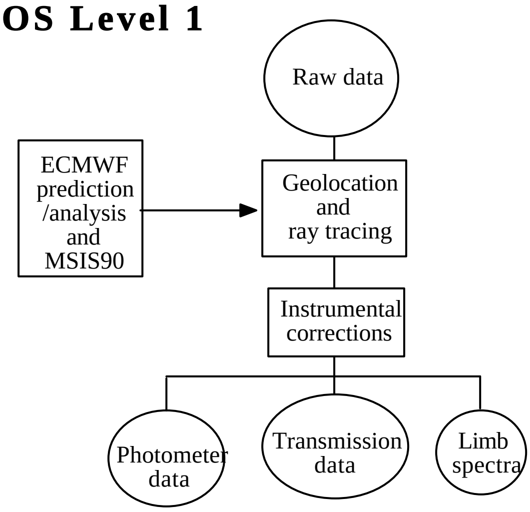
Global **O**zone **M**onitoring by **O**ccultations of **S**tars



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

GOMOS Level 1



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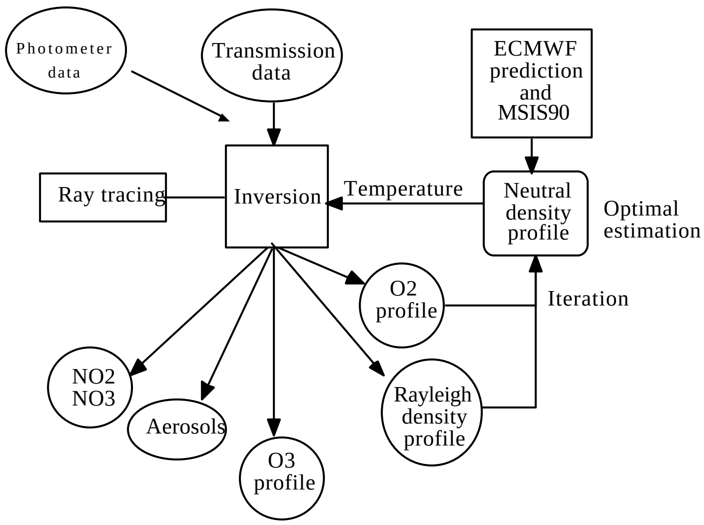
GOMOS inversion simplified: Level 2



When we were young

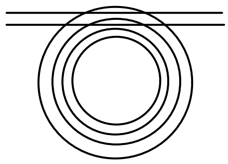
$$\frac{I_{meas}(z,\lambda)}{I_{star}(\lambda)} = T(\lambda) = e^{-\sigma(\lambda)N(z)}$$ Beer's law

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

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

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

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



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

Transmission model for extinction

Transmission data to be compared
to the model transmission

$$T_{mod}(\lambda_k, t_j)= d\lambda W(\lambda-\lambda_k,t)e^{-\Sigma\ \sigma(\lambda,T(s))\,\rho_j(s)\ ds}$$

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:

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

Separate spectral and vertical inversions

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

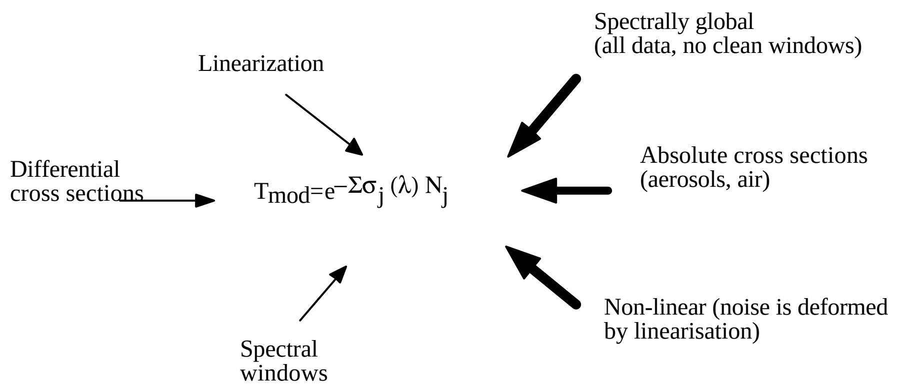
$$=\Sigma\sigma_j^{eff}(\lambda)N_j$$ separation of spectral and vertical problem

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

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

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

Spectral inversion: uvis spectral inversion possibilities



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Spectral inversion

We aim to minimize

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

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

Solution by Levenberg-Marquard algorithm

Residual=T$_{model}$-T$_{observed}$

Movie not included in this version

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GOMOS

Minimize

$$(T_{mittaus}(\lambda) - e^{-\sigma_{otsoni}(\lambda)N_{otsoni} - \sigma_{NO2}(\lambda)N_{NO2}})^2 \longrightarrow N_{otsoni}, N_{NO2}$$

Interaction not included in this version

Movie not included in this version

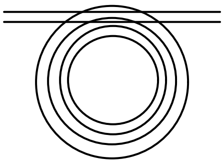
Experiment
(© P. Pirjola)

Levenberg-Marquardt
(© J. Tamminen)

Vertical inversion

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

Discretization of the atmsphere into layers:



$N = \Sigma \rho(s_i)\, \Delta s_i$

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

$\mathbf{N} = K\mathbf{r}$

which can be solved in standard methods.

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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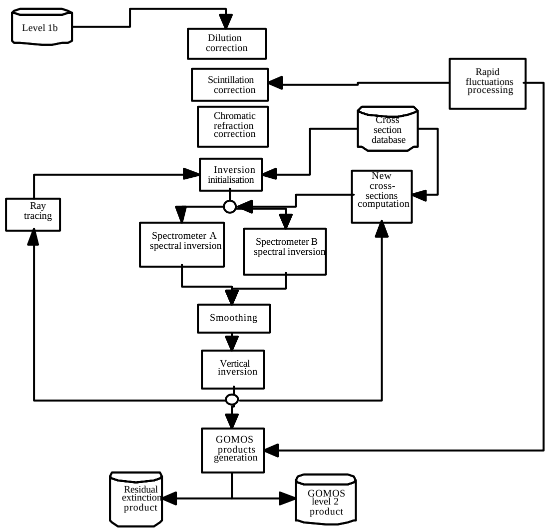
Iteration: Gomos atmosphere

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)

Level 2 architecture



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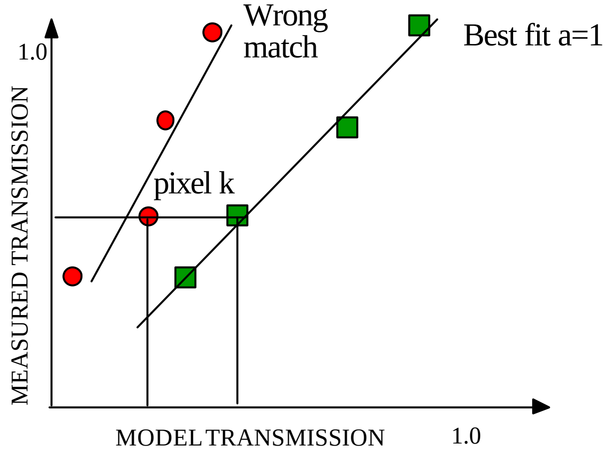
IR SPECTRAL INVERSION

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 H2 O):

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

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



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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.

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

From the refraction angle we can find the refractive index

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

Finally the neutral density is given by

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

and the high resolution temperature can be calculated

Consistency

1. In Level 1 the atmosphere (density and temperature) is formed from:
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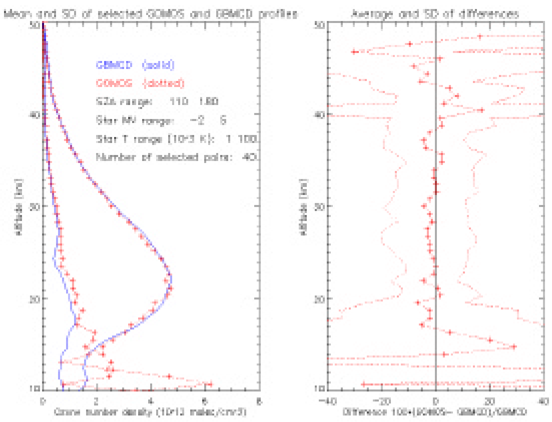
Statistical comparison for lidars (40 cases)



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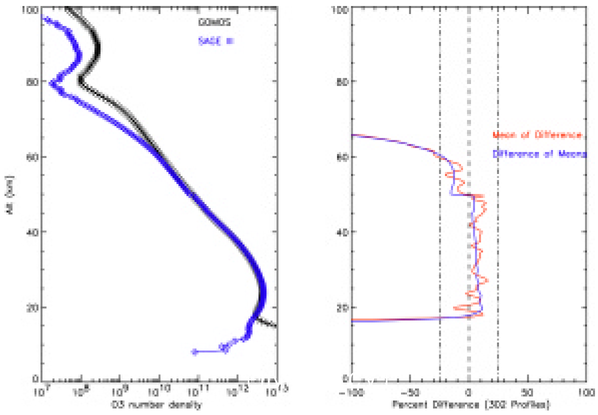
GOMOS ozone validation: GOMOS vs SAGE III



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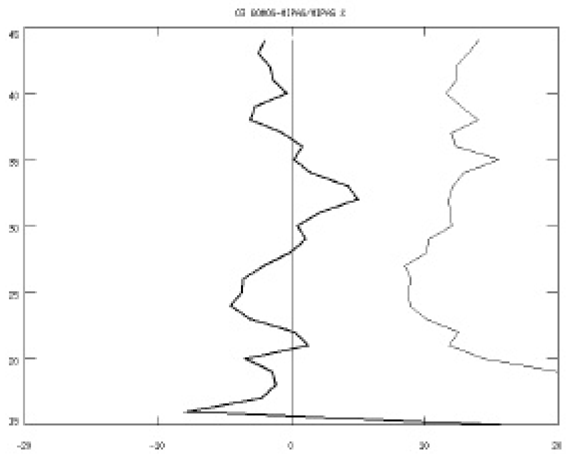
GOMOS ozone validation: GOMOS vs MIPAS



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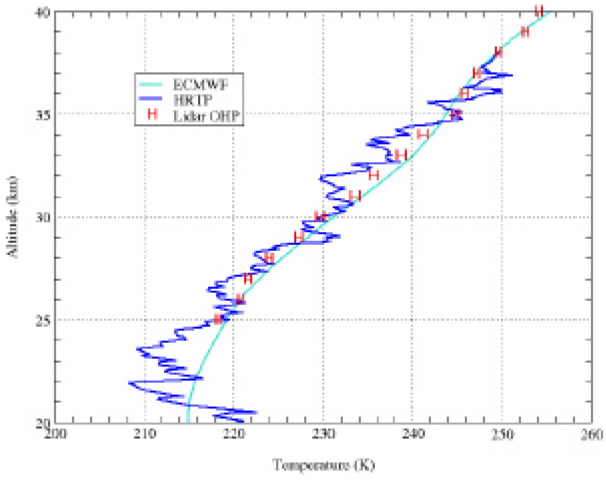
GOMOS high resolution T vs ECMWF and lidar



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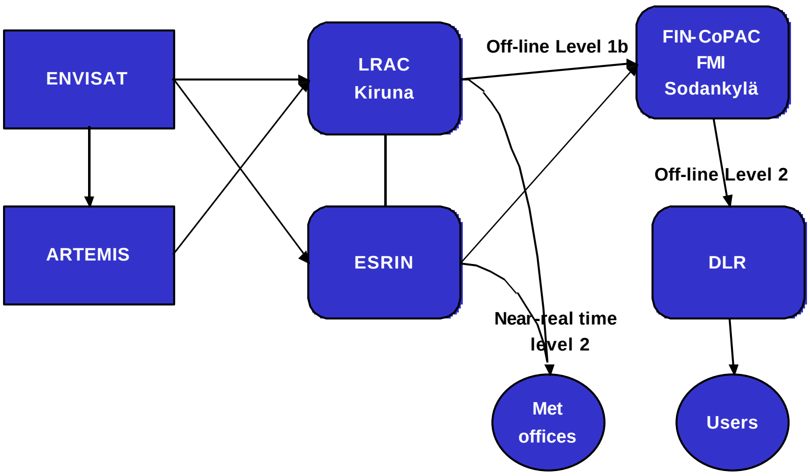
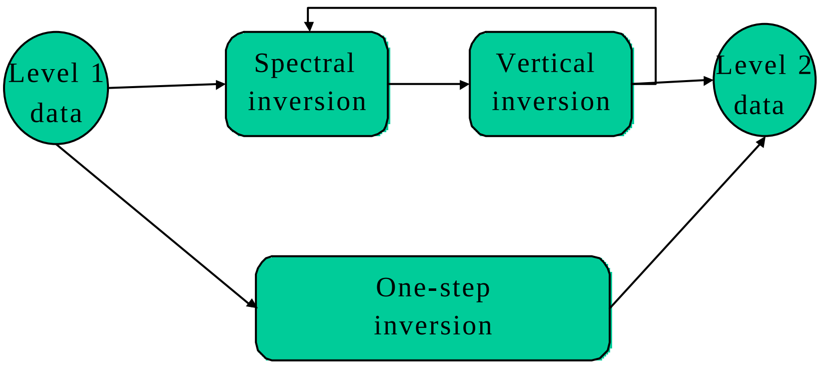
GOMOS data flow



Future developments: one-step



No of wavelengths=1500
Number of layers=70
i.e. 105000 data points

No of gases=5
Number of layers=70
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

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

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?

$<m> = P(m|d)\ m\ dm$

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

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

$P(m|d) = e^{-(m-<m>)^T Q(m-<m>)/2}$

For others:

-are there multiple minima, flat regions, valleys, ridges?

-what are "good" estimators for complicated distributions?

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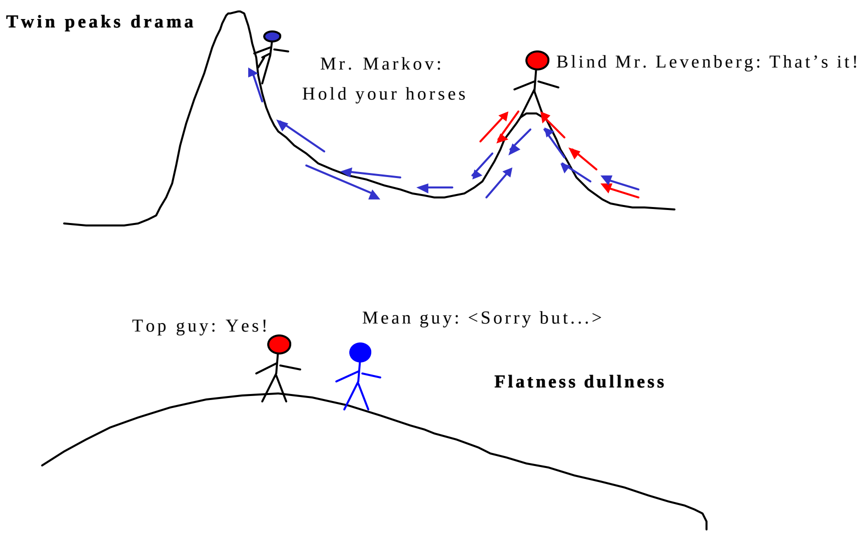
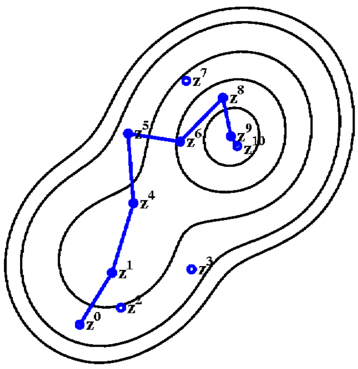
Ultimate estimators: Markov chain Monte Carlo



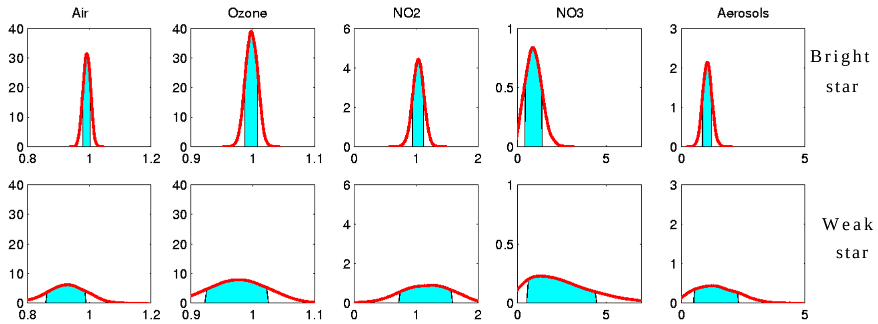
Markov chain Monte Carlo



Estimators from MCMC

$$\langle x_i \rangle = \frac{1}{N}\sum_{t}^{N} z_i^t$$

MCMC examples



Marginal posterior distributions at 30 km for different gases

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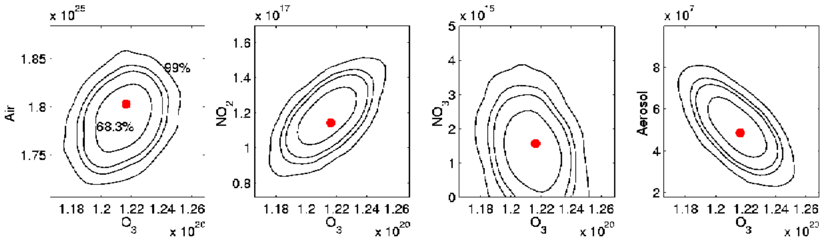
MCMC examples



Marginal two-dimensional posterior distributions at 30 km for different gases

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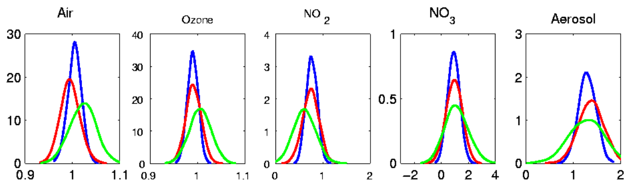
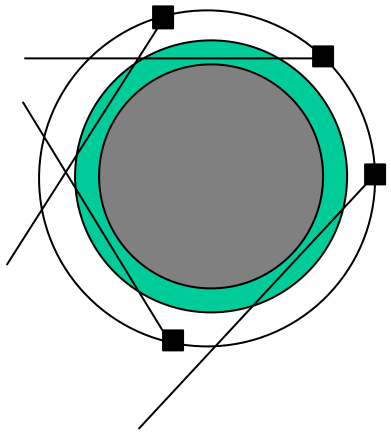
Measurement or retrieval design by MCMC



Marginal posterior distributions for different gases with varying number of spectral data. Blue: 1417 wavelengths, red: every second, green: everey fourth

Determination of model dimension: **Reversible jump MCMC**
Examples: what absorbers, what kind of aerosol model

Atmospheric tomography



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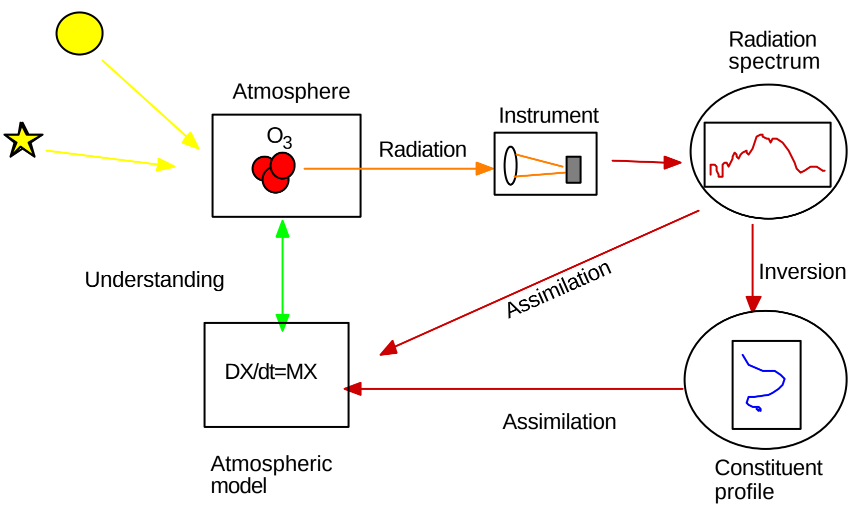
GOMOS

Inversion-Assimilation



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/