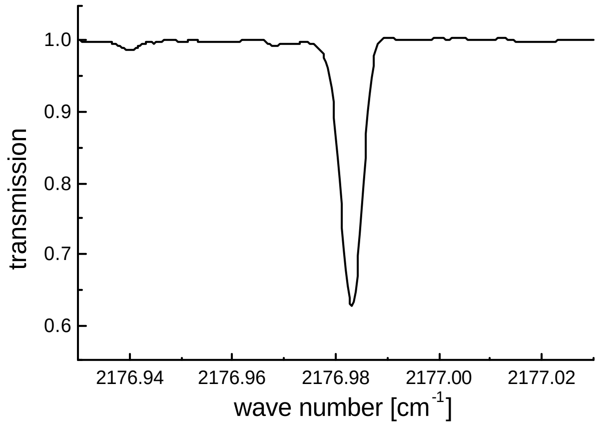
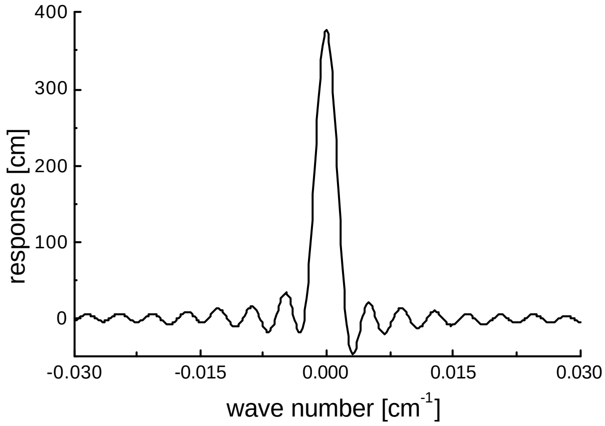
LINEFIT concept

Problem: Transition from measured transmission spectrum to ILS





Necessary steps:

- Calculation of irradiated spectrum
- Deconvolution of ILS

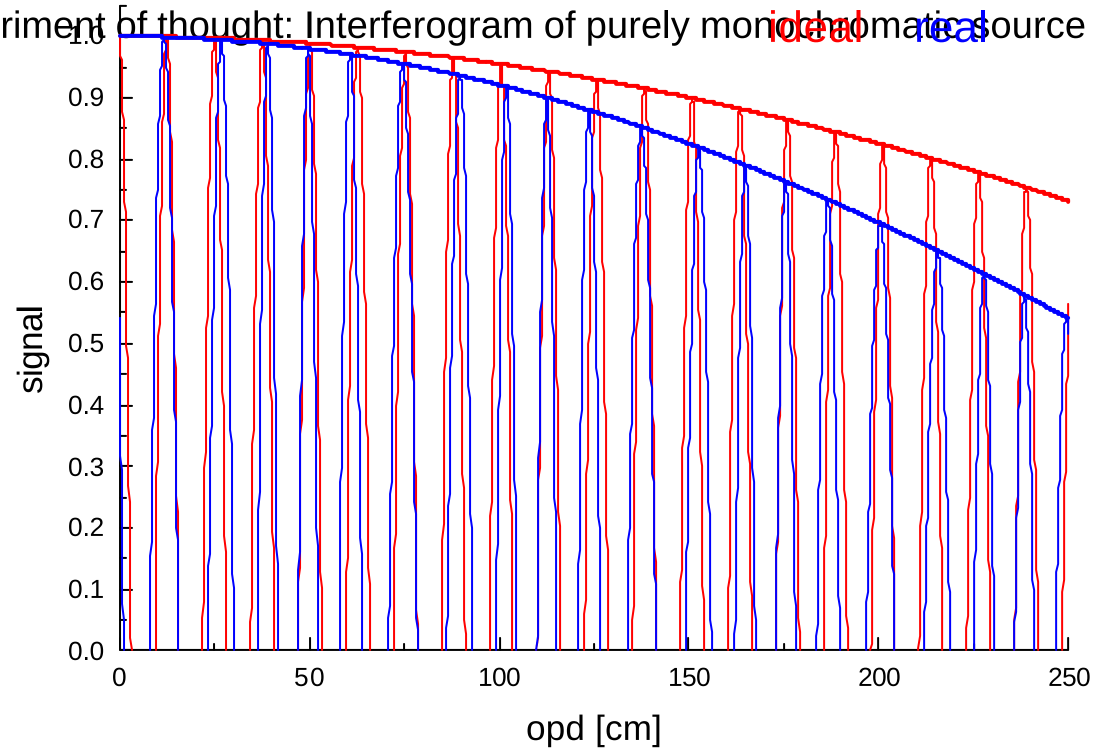
  Direct deconvolution is unsatisfactory due to comparable width of ILS and signatures in the irradiated spectrum and due to presence of noise.

Solution:

Introduce a model of the ILS and do a fit of model parameters. For optimal reconstruction use sufficient number of parameters and appropriate (physically motivated) regularisation constraint.

ILS parameterisation used by LINEFIT

Experiment of thought: Interferogram of purely monochromatic source



The ideal (phase corrected) interferogram shows pure cosine oscillation embedded in a sinc-shaped envelope. The actual (phase corrected) interferogram shows deviating modulation and phase orientation: Representation by complex modulation efficiency (Note ambiguity: Linear phase error equivalent to shift in spectral domain).

LINEFIT simple ILS model parameters:

Linear decline of modulation efficiency, constant phase error

LINEFIT extended ILS model parameters:

complex modulation efficiency at 20 equidistant positions along optical path difference. Regularisation constraints are: Assume constant phase error, assume constant modulation efficiency. LINEFIT8: User defined constraints possible!

Additional parameters to be fitted

LINEFIT handles several MWs at the same time to deduce a common ILS.

Each MW should contain a single, isolated line.

For each MW there are two (up to four) additional fit parameters:

- Individual spectral shift

  To compensate for imperfect calibration of spectral abscissa and imperfect spectroscopic data

- Individual gas column

  To compensate for error in gas temperature and imperfect spectroscopic data

- LINEFIT8: Individual scale and slope of transmission spectrum

  To compensate for errors in the preparation of transmission spectrum

  (Note: Careful adjustment by hand using a wider spectral window is an accurate method. If you prefer to do joint fit of these quantities using LINEFIT, choose MW wider than in case of ILS retrieval alone, at least 0.2 cm^{-1}.)

The retrieval procedure

For each parameter to be adjusted, LINEFIT calculates a derivative (generally constructed numerically). The "derivative spectra" build up the Jakobian A. The linearised problem is solved, several iterations are needed to find the final solution (number of iterations set by user).

- Retrieval in case of simple parameter set

  Number of parameters: 2 + 2 n_{MW} (+ 2 n_{MW})

  Problem is well-posed, no additional constraints needed

  $$\vec{f}^{\,i+1} = \vec{f}^{\,i} + (A^{i,T} A^{i})^{-1} A^{i,T} (\vec{T}_{mess} - \vec{T}^{\,i}_{calc})$$

- Retrieval in case of extended parameter set

  Number of parameters: 40 + 2 n_{MW} (+ 2 n_{MW})

  Problem is ill-posed, regularisation constraints needed

  $$\vec{f}^{\,i+1} = (A^{i,T} A^{i} + g^{2}_{\mathrm{mod}} B^{T}_{2,\mathrm{mod}} B_{2,\mathrm{mod}} + g^{2}_{phas} B^{T}_{2,phas} B_{2,phas})^{-1} A^{i,T} ((\vec{T}_{mess} - \vec{T}^{\,i}_{calc}) + A^{i} \vec{f}^{\,i})$$

  cost function $\left|\vec{T}_{mess} - \vec{T}_{calc}\right|^{2} + g^{2}_{\mathrm{mod}} \left|B_{2,\mathrm{mod}} \vec{f}^{\,i}_{\mathrm{mod}}\right|^{2} + g^{2}_{phas} \left|B_{2,phas} \vec{f}^{\,i}_{phas}\right|^{2}$

  LINEFIT8:

  $$\vec{f}^{\,i+1} = (A^{i,T} A^{i} + \sum_{j=1}^{2} g^{2}_{j,\mathrm{mod}} B^{T}_{j,\mathrm{mod}} C^{T}_{j} C_{j} B_{j,\mathrm{mod}} + \sum_{j=1}^{2} g^{2}_{j,phas} B^{T}_{j,phas} C^{T}_{j} C_{j} B_{j,phas})^{-1} A^{i,T} ((\vec{T}_{mess}$$

  $$- \vec{T}^{\,i}_{calc}) + A^{i} \vec{f}^{\,i} + \sum_{j=1}^{2} g^{2}_{j,\mathrm{mod}} B^{T}_{j,\mathrm{mod}} C^{T}_{j} C_{j} B_{j,\mathrm{mod}} \vec{f}^{\,reg}_{\mathrm{mod}} + \sum_{j=1}^{2} g^{2}_{j,phas} B^{T}_{j,phas} C^{T}_{j} C_{j} B_{j,phas} \vec{f}^{\,reg}_{phas})$$

B_1 = operator for deviation, B_2: Operator for first derivative, $C_{1/2}$: path dependent weight of each constraint. Cost function:

$$\left|\vec{T}_{mess} - \vec{T}_{calc}\right|^2 + \sum_{j=1}^{2} g_{j,\mathrm{mod}}^2 \left|C_j B_{j,\mathrm{mod}} (\vec{f}_{\mathrm{mod}}^{\,i} - \vec{f}_{\mathrm{mod}}^{\,reg})\right|^2 + \sum_{j=1}^{2} g_{j,phas}^2 \left|C_j B_{j,phas} (\vec{f}_{phas}^{\,i} - \vec{f}_{phas}^{\,reg})\right|^2$$

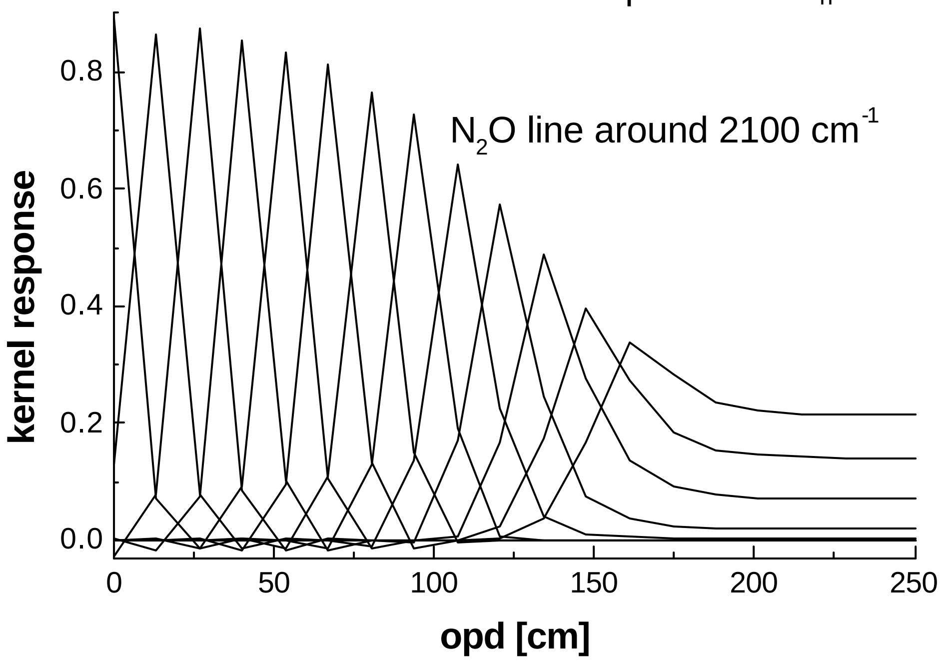
Significance of results

Measured spectral lines and ILS are of comparable width. Therefore results a reduced visibility of details in the modulation efficiency and phase orientation at larger OPD. The significance of the retrieved parameter vector is represented by the averaging kernels.

$$\frac{\partial \vec{f}_{reg}}{\partial f_n} = K \vec{e}_n$$

$$K = (A^T A + g_{\mathrm{mod}}^2 B_{\mathrm{mod}}^T B_{\mathrm{mod}} + g_{phas}^2 B_{phas}^T B_{phas})^{-1} A^T A$$

The column n of the averaging kernel matrix K depicts the response of the retrieved parameter vector to the variation of the model parameter f_n.



Note: Details in modulation and phase beyond the limit accessible by gas cell measurements are hardly detectable in atmospheric observations also. Therefore, this is no painful limitation of cell measurements. Also read LINEFIT kernels the other way round: Useful resolving power for measuring atmospheric lines (comparable Doppler width, comparable SNR) can be estimated from the kernels.