Transformation of irradiated to measured spectral distribution due to finite spectral resolution and field of view extent of a Fourier transform spectrometer

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Abstract: It is described how instrumental effects on the irradiated spectrum (apodized instrumental line shape, noise, field of view, spectral shift) are simulated by KOPRA. The calculation of derivatives with respect to elevation, spectral shift, ordinate offset, ordinate scale, and instrumental line shape parameters is presented.

1 Introduction

Any real spectrometer has limited spectral resolution and thereby acts as a low pass filter on the irradiated spectral distribution. The measured spectrum can be described locally as the convolution of the incoming spectrum with an appropriate instrumental line shape (ILS). KOPRA performs the convolution with a truncated ILS in the spectral domain using an interpolatoric integration rule.
In case of a Fourier transform spectrometer the ILS is the Fourier transform of the modulation efficiency in the interferogram domain. Thereby the natural ILS assuming constant modulation efficiency up to maximal optical path difference L is the sinc function. In a real instrument the modulation efficiency decreases somewhat with increasing optical path difference due to finite acceptance angle of the interferometer (called self-apodisation). Interferometric misalignment, aberrations in the optical system and imperfect phase correction further distort the ILS and destroy its symmetry. The general ILS is the Fourier transform of a complex valued and wavenumber dependent modulation efficiency.
A multiplicative weighting function working in the interferogram domain can be used to modify the resulting AILS. This procedure is called numerical apodisation. To reduce the sidelobes of the raw ILS, a variety of apodisation functions are in use. KOPRA calculates the AILS from the resulting modulation efficiency in the interferogram domain (including self -apodisation) and handles all common apodisation functions. Instrumental imperfection can be described in terms of a set of 2 parameters: an additional linear modulation loss and a phase error. Derivatives of the spectrum with respect to these parameters can be calculated. In case of MIPAS ENVISAT the ILS model given by BOMEM is used by KOPRA. Alternatively, KOPRA can use an external ILS given in tabulated form.
Any real spectrometer accepts radiation out of a finite solid angle. It acts as a low pass filter on the irradiated spectral distribution with respect to directional variability. The instrumental responsitivity to a point source in infinity as a function of its orientation with respect to the instrumental line of sight characterises the *external* field of view (FOV). The irradiated spectral distribution has to be convolved with this sensitivity function. Since in a Fourier Transform spectrometer the optical path difference depends on the inclination of the wavefront in the interferometer, inhomogenous illumination of the FOV affects the spectral response also. This effect is small in typical situations of remote sensing and KOPRA allows to estimate it. For this purpose, obviously the FOV inside the interferometer (*internal* FOV) has to be used.
In the retrieval process, derivatives to each of the fit parameters are needed. In the context under consideration here KOPRA offers derivatives with respect to

- line of sight (LOS)
- spectral shift
- ordinate scale
- ILS parameters: linear modulation loss and phase error
- BOMEM ILS parameters: retroreflector linear shear variation along z-axis and IR misalignment along y direction

KOPRA offers a noise generator. If no numerical apodisation is performed, the generated Gaussian noise is uncorrelated on a spectral grid of width 1/2L. If numerical apodisation is performed and/or grid spacing differs from 1/2L, the correlations reproduce the statistical behaviour resulting from white Gaussian noise in interferogram domain.

2 Calculation of AILS

KOPRA determines a single sided ($x \geq 0$) and complex-valued modulation efficiency with symmetric real and antisymmetric imaginary parts. The AILS is the Fourier transform of the modulation efficiency. The modulation efficiency $M(x)$ includes the numeric apodisation function, the modulation loss due to self apodisation, the linear modulation loss and the phase error.

$$M(x) = M_{resolution}(x) \times M_{numeric}(x) \times M_{self}(x) \times M_{linear}(x) \times M_{phase}(x) \quad (1)$$

- resolution

  The interferogram is restricted to maximal optical path difference L

  $M_{resolution}(x) = 1 \quad \text{if} \quad |x| \leq L$
  $M_{resolution}(x) = 0 \quad \text{else}$

- apodisation function

  (a) sinc
  $M_{numeric} = 1$

  (b) triangle
  $M_{numeric} = 1 - |x|/L$

  (c) Hamming
  $M_{numeric} = 0.53856 + 0.46144 \times \cos(\pi \times x/L)$

  (d) Blackmann-Harris 3-term
  $M_{numeric} = 0.42323 + 0.49755 \times \cos(\pi \times x/L) + 0.07922 \times \cos(2 \times \pi \times x/L)$

  (e) Blackmann-Harris 4-term
  $$M_{numeric} = 0.35875 + 0.48829 \times \cos(\pi \times x/L) + 0.14128 \times \cos(2 \times \pi \times x/L) + 0.01168 \times \cos(3 \times \pi \times x/L)$$

  (f) Norton-Beer weak
  $M_{numeric} = 0.384093 - 0.087577 \times \left(1 - (x/L)^2\right) + 0.703484 \times \left(1 - (x/L)^2\right)^2$

  (g) Norton-Beer medium
  $M_{numeric} = 0.152442 - 0.136176 \times \left(1 - (x/L)^2\right) + 0.983734 \times \left(1 - (x/L)^2\right)^2$

  (h) Norton-Beer strong
  $M_{numeric} = 0.045335 - 0.554883 \times \left(1 - (x/L)^2\right)^2 + 0.399782 \times \left(1 - (x/L)^2\right)^4$

- self apodisation

  The interferometer has finite acceptance angle. It can be shown, that optical path difference depends on the inclination of the wavefront versus the optical axis. In case of homogeneously illuminated circular internal FOV of semidiameter one finds that this leads to an additional loss of modulation:

  $M_{self} = \frac{\sin(\pi \times \Delta\nu \times x)}{\pi \times \Delta\nu \times x}$ with $\Delta\nu = 0.5 \times \nu \times \alpha^2$

  Note that the self apodisation (and thereby the resulting AILS) depends on spectral position ν. The additional modulation loss describes the consequences of the finite acceptance angle not completely. In addition, the spectral abscissa is scaled by $0.5 \times (\cos(\alpha) + 1)$. Since the latter effect is usually absorbed in the spectral calibration, KOPRA *does not perform any spectral scaling or shift on the calculated spectrum due to self apodisation.*

- linear modulation loss

  This term is used to model the width of the imperfect AILS.

  $M_{linear} = 1 - (1 - a) \times x/L$

  the factor a gives the modulation efficiency at maximal path difference vs ideal instrument.

- phase error

  This term is used to model the asymmetry of the imperfect AILS. The phase error φ is given in radians.

  $M_{phase} = \frac{e^{-i\varphi}}{\cos(\varphi)}$

  The norm of the AILS is fixed by the real part of $M(0)$. The denominator ensures the norm to be unity.

Since the real valued AILS is the Fourier transform of the complex-valued modulation efficiency, the latter is symmetric in the real part and antisymmetric in the imaginary part. Due to this symmetry, the AILS is fully determined by a single sided modulation efficiency interferogram.
KOPRA uses a semianalytic discrete Fourier transform. This method avoids channeling effects and facilitates fast and accurate calculation of the AILS on any grid spacing. The values of the modulation efficiency are calculated at N equidistant optical path differences x_i up to maximal path difference L

$$x_i = \frac{N - i}{N - 1} \times L \qquad \text{with} \quad i = 1, 2, \cdots, N$$

It is assumed, that in between these positions the modulation efficiency can be approximated by linear interpolation to sufficient accuracy. KOPRA uses $N = 200$. This interferogram can be transformed analytically, by breaking both real and imaginary part down into a boxcar and N-1 triangles and adding up the Fourier transforms of these functions. The width of the boxcar is $x_1 = L$ and the widths of the triangles are $x_1, x_2, \cdots, x_{N-1}$. The contribution of the real-part boxcar $g_{box,re}$ is

$$g_{box,re} = Re(M(x_N))$$

and the contribution of the real-part triangle $g_{triang,re}$ to x_i is

$$\begin{aligned} g_{triag,re}(i) &= (N + 1 - i) \times Re(M(N + 1 - i) - M(N + 2 - i)) \\ &\quad - \sum_{k=2}^{i-1} g_{triang,re}(k)/(N + 1 - k) \end{aligned}$$

The contributions for the imaginary-part boxcar and triangles are found accordingly by exchanging real by imaginary parts in the formulas. To achieve a compact notation, we use $k = 2 \times \pi \times \nu$ in the following. Note that the analytic Fourier transforms given below are normalized to unity with respect to the wavenumber abscissa ν.
The Fourier transform of the real-part boxcar is:

$$FT_{box,re}(k, L) = \frac{2 \times \sin(k \times L)}{k}$$

The Fourier transform of the imaginary-part boxcar is:

$$FT_{box,im}(k, L) = \frac{4 \times \sin^2(0.5 \times k \times L)}{k}$$

The Fourier transform of the real-part triangle of width x_i is:

$$FT_{triag,re}(k, x_i) = \frac{4 \times \sin^2(0.5 \times k \times x_i)}{x_i \times k^2}$$

The Fourier transform of the imaginary-part triangle of width x_i is

$$FT_{triag,im}(k, x_i) = \frac{2 \times (x_i \times k - \sin(x_i \times k))}{x_i \times k^2}$$

The AILS then is given by superposition of all analytic contributions:

$$\begin{aligned} AILS(k) &= g_{box,re} \times FT_{box,re}(k, L) + \sum_{i=1}^{N-1} g_{triag,re}(i) \times FT_{triag,re}(k, x_i) \\ &\quad + g_{box,im} \times FT_{box,im}(k, L) + \sum_{i=1}^{N-1} g_{triag,im}(i) \times FT_{triag,im}(k, x_i) \end{aligned}$$

3 AILS Model for MIPAS-ENVISAT

KOPRA uses the semiempiric BOMEM ILS model to construct the AILS of the MIPAS instrument onboard ENVISAT. This model is discussed in detail in PO-RS-DOG-GS-0002. A complex modulation efficiency is calculated:

$$\begin{aligned} M(\nu, x) &= M_{IR}(\nu, x) \times M_L(\nu, x) \times M_V(\nu, x) \times M_{SP}(\nu, x) \times M_{Ld}(\nu, x) \\ &\quad \times M_{Lw}(\nu, x) \times M_{Lf}(\nu, x) \times M_{Res}(x) \times M_{numeric}(x) \end{aligned}$$

M_{IR}	complex modulation function related to IR-misalignment
M_L	complex modulation function related to laser misalignment
M_V	complex modulation function related to optical speed
M_{SP}	complex modulation function related to sampling distortions at turn around
M_{Ld}	complex modulation function related to laser drift
M_{Lw}	real modulation function related to white noise of laser
M_{Lf}	real modulation function related to 1/f noise of laser
M_{Res}	real modulation function related to limited optical path difference
$M_{numeric}$	real modulation function related to numerical apodisation (Norton-Beer strong)

These modulation functions depend on 24 parameters. Their values are specified by the user in the KOPRA input file. Two out of these are designated to describe AILS imperfections. They are marked with asterisks.

(a) maximal optical path difference [nominal/default value: 20 cm]

(b) infrared misalignment y-direction [nominal/default value: 0 rad] *

(c) infrared misalignment z-direction [nominal/default value: 2×10^{-4}rad]

(d) retroreflector linear shear along y [nominal/default value: 4×10^{-3}cm]

(e) retroreflector linear shear along z [nominal/default value: 4×10^{-3}cm]

(f) linear shear variation along y [nominal/default value: 0 , dimensionless]

(g) linear shear variation along z [nominal/default value: 0 , dimensionless] *

(h) full interferometer divergence along y [nominal/default value: 5.4×10^{-3}rad]

(i) full interferometer divergence along z [nominal/default value: 9.0×10^{-3}rad]

(j) blur angular width along y [nominal/default value: 5.2×10^{-4}rad]

(k) blur angular width along z [nominal/default value: 3.3×10^{-4}rad]

(l) laser misalignment along y [nominal/default value: 1.5×10^{-4}rad]

(m) laser misalignment along z [nominal/default value: 1.5×10^{-4}rad]

(n) optical speed of interferometer [nominal/default value: 10.0 cm/s]

(o) initial sampling pertubation [nominal/default value: 4×10^{-8}cm]

(p) time constant of exponential attentuation of initial sampling pertubation [nominal/default value: 0.16 s]

(q) time constant of exponential attentuation of initial speed fluctuation [nominal/default value: 0.016 s]

(r) initial relative speed fluctuation at beginning of scan [nominal/default value: 0.03, dimensionless]

(s) gain slope of IR electrical response [nominal/default value: -0.22, dimensionless]

(t) mismatched delay between electronic response and ADC trigger [nominal/default value: 1.4×10^{-6}s]

(u) laser wavenumber [nominal/default value: 7692.0 cm^{-1}]

(v) relative drift rate of laser wvnr [nominal/default value: 1.0×10^{-8}, dimensionless]

(w) bandwith laser white noise [nominal/default value: 2×10^{7}Hz]

(x) bandwith laser 1/f noise [nominal/default value: 0 Hz]

To avoid confusion, it is important to mention that the BOMEM ILS model and the KOPRA AILS model described above introduce complex modulation functions with different meaning. The KOPRA modulation function is just the inverse transform of a real AILS. The symmetry properties of the modulation function guarantee the imaginary part of the AILS to be zero. The BOMEM modulation function has a physical meaning: it characterises amplitude and phase orientation of the modulation related to a monochromatic input signal. The ILS is proportional to the real part of the Fourier transform of the modulation function.
KOPRA handles the BOMEM model in the following way: The double-sided modulation function $M(\nu, x)$ is calculated as given in document PO-RS-DOG-GS-0002. Then $M(\nu, x)$ is scaled and rotated in the complex plane to achieve a real $\tilde{M}(\nu, 0)$ normalised to unity at zero path difference:

$$\tilde{M}(\nu, x) = M(\nu, x) \times e^{-i\varphi}/|M(\nu, 0)| \qquad \text{with} \qquad M(\nu, 0) = |M(\nu, 0)| \times e^{i\varphi}$$

A single sided modulation function $\tilde{\tilde{M}}(\nu, x)$ is calculated from $\tilde{M}(\nu, x)$ with symmetric real and antisymmetric imaginary part.

$$\tilde{\tilde{M}}(\nu, x) = 0.5 \times (Re(\tilde{M}(\nu, x) + \tilde{M}(\nu, -x)) + i \times Im(\tilde{M}(\nu, x) - \tilde{M}(\nu, -x)))$$

The Fourier transform of $\tilde{\tilde{M}}(\nu, x)$ is the ILS. It is performed using the semianalytic discrete transform described above.

4 Convolution

The measured spectrum $\tilde{S}(\nu)$ is the convolution of the irradiated spectrum $S(\nu)$ with the instrumental lineshape $AILS(\nu - \nu_0)$.

$$\tilde{S}(\nu_0) = \int S(\nu) \times AILS(\nu_0 - \nu) d\nu \qquad \text{with} \qquad \int AILS(\nu) d\nu = 1$$

The AILS transmits the incoming flux at spectral position ν to measured flux at spectral position ν_0. Despite the fact, that the AILS is a function of ν it is assumed that all significant contributions to the measured flux at ν_0 are transmitted by the AILS strictly valid only at position ν_0. Moreover, the measured flux is usually calculated in a whole microwindow extending from ν_1 to ν_2. KOPRA then uses the AILS valid for the arithmetic mean wavenumber $0.5 \times (\nu_1 + \nu_2)$. In the practice of remote sensing, the first approximation is always justified. The second approximation demands $|(\nu_1 - \nu_2)|/(\nu_1 + \nu_2) \leq 0.02(0.1)$ as a rule of thumb for a negligible variation of modulation efficiency of 0.01 (0.05) at maximal path difference.
Since the calculation of $S(\nu)$ has to be restricted to a finite interval, the integral has to be truncated. The modification must not be done in the following way

$$\tilde{S}(\nu_0) = \int S(\nu) \times AILS(\nu_0 - \nu) \times W(\nu_1, \nu_2) d\nu$$

$$\begin{array}{lll} \text{with} & W(\nu_1, \nu_2) = 1 & \text{if} \quad (\nu - \nu_1)(\nu - \nu_2) < 0 \\ & W(\nu_1, \nu_2) = 0 & \text{if} \quad (\nu - \nu_1)(\nu - \nu_2) \geq 0 \end{array}$$

because this is equivalent to the convolution of the untruncated AILS with the windowed spectrum $S(\nu) \times W(\nu_1, \nu_2)$. The sharp boarders of the window give rise to the Gibbs phenomenon: unwanted oscillations spread from the boarders into the spectrum.
To avoid these oscillations, KOPRA calculates the spectrum in an enlarged interval extending from $\nu_{1e} = \nu_1 - \Delta\nu$ to $\nu_{2e} = \nu_2 + \Delta\nu$ and the truncation is assigned to the AILS

$$\begin{aligned} \tilde{S}(\nu_0) &= \int_{\nu_0 - \Delta\nu}^{\nu_0 + \Delta\nu} S(\nu) \times L(\nu_0 - \nu) d\nu \\ &= \int S(\nu) \times AILS(\nu_0 - \nu) \times W(\nu_0 - \Delta\nu, \nu_0 + \Delta\nu) d\nu \end{aligned}$$

KOPRA chooses the truncation window according to the users specification to ensure that the transmission $T(\nu) = AILS(\nu)/AILS(0)$ from outside the window is lower than a certain threshold. Due to the truncation, the norm of the AILS is slightly lower than unity (see Table 4).
KOPRA solves the radiative transfer equation at a finite number of discrete spectral positions. The calculated incoming spectrum is interpolated to an equidistant spectral grid before the convolution is performed. The grid spacing has to be dense enough to depict even the sharpest details to be expected in the spectrum. In the atmospheric spectrum, these are the cores of purely Doppler-broadened lines. The hwhm γ_D of a line at spectral position ν emerging from a species of mass m in an atmospheric layer of temperature T is

$$\begin{aligned} \gamma_D &= \sqrt{\frac{2kT}{m}} \times \frac{1}{c \ln 2} \times \nu \\ \gamma_D \left[cm^{-1}\right] &\approx 6.22 \times 10^{-7} \times \sqrt{\frac{T[K]}{m[amu]}} \times \nu \left[cm^{-1}\right] \end{aligned}$$

Apodisation	T=0.01	T=0.001	T=0.0001
boxcar	16/L	160/L	1600/L
	0.9957	0.9996	1.000
triangle	3/L	10/L	32/L
	0.9666	0.9899	0.9968
Hamming	1/L	23/L	510/L
	1.0029	0.9997	1.0000
3-term Blackmann-Harris	1.5/L	2/L	17/L
	0.9999	1.0000	0.9999
4-term Blackmann-Harris	2/L	2.5/L	14/L
	0.9998	0.9999	0.9999
Norton-Beer weak	9/L	85/L	860/L
	0.9971	0.9997	1.0000
Norton-Beer medium	4/L	40/L	510/L
	0.9977	0.9997	1.0000
Norton-Beer strong	1.5/L	14/L	140/L
	1.0005	0.9997	1.0000

Table 1: Truncation radius for AILS and norm of truncated AILS (no self-apodisation). L denotes the maximal optical path difference.

If higher atmospheric layers contribute noticeably in the spectrum, the user defined fine grid spacing should not exceed γ_D. In a strict sense, a sampling dense enough to determine the continuous function $S(\nu)$ exactly is impossible, because the incoming spectrum is *not bandwith limited*! In practice, the KOPRA user should determine a sufficient sampling density for the defined situation by a control run using halved spacing.
In case of a Fourier transform spectrometer, the highest detectable sinusoidal modulation in the irradiated spectrum is determined by the maximal optical path difference of the instrument L. The limiting spectral modulation along the wavenumber abscissa is then given by 1/L. Therefore, according to the sampling theorem, the gridpoint density in the measured spectrum must be at least 1/2L. *Because the measured spectrum is bandwith limited*, the continuous function $\tilde{S}(\nu)$ is then completely determined.
KOPRA combines the convolution with the reduction of gridpoint density. The convolution integral is evaluated on the user defined output grid. The simplest interpolatoric integration rule is applied:

$$\tilde{S}(\nu_i) = \int S(\nu) \times AILS(\nu_i - \nu) d\nu \approx \Delta\nu \times \sum_{n=-N}^{N} AILS(n) \times S(i-n)$$

The spectral stepwidth is denoted by $\Delta\nu$. Since the integrand is localised (tends to zero near the boarders of the integration interval), the accuracy of the result cannot be enhanced substantially by means of any higher polynomial integration rule.

5 Noise Generator

KOPRA offers a noise generator. In case of a Fourier transform spectrometer, it is usually assumed that the noise is Gaussian and independent from sampling position in the interferogram. We follow this assumption here, because noise contributions

of differing statistical behaviour are highly instrument and scene specific.
The irradiated spectrum calculated by KOPRA is interpolated to an equidistant fine grid spacing before the convolution with the AILS is performed (see section 'convolution'). KOPRA introduces the noise in the spectral domain: the statistically independent Gaussian noise is generated on this same fine grid. This noise is convolved with an appropriate AILS_{noise} and thereby adopts the correct statistical properties found in the measured spectrum. Note that the AILS to be applied to the irradiated spectrum and AILS_{noise} are *not identical.* The latter does incorporate neither self-apodisation nor modulation loss due to misalignment (see section 'Calculation of AILS'), because the variation of modulation efficiency with optical path difference does not affect the noise level, which depends on total photon number and detector characteristics.
The statistically independent Gaussian noise of standard deviation σ_f on the fine grid is calculated using

$$y = \sigma_f \times \cos(2 \times \pi \times x_1) \times \sqrt{-2 \times log \times x_2}$$

with evenly distributed random numbers $x_1, x_2 \in \{0, 1\}$. KOPRA uses the standard Fortran 90 calling sequence for random numbers. Since no standard algorithm is defined by the language, the quality of the random numbers generated may depend on the computer and compiler used.
The convolution with AILS_{noise} mixes the statistically independent sample points. If no numerical apodisation is performed, AILS_{noise} is the sinc-function to maximal optical path difference L. The distance between two independent sample points is enlarged from the fine grid spacing $\Delta\nu$ to 1/2L. Due to this smoothing, the standard deviation on the coarse grid σ_c is reduced:

$$\sigma_c = \sigma_f \times \sqrt{2 \times \Delta\nu \times L}$$

The KOPRA user specifies σ_c measured at each sample point in the resulting spectrum assuming a sinc-shaped AILS_{noise}. If numeric apodisation is performed, the standard deviation at each sample point in the resulting spectrum is smaller than σ_c. This convention is advisable, because it keeps the quality of the measurement constant when comparing the retrieval quality using different kinds of apodisation functions.

6 Field of View (FOV)

If the radiation field shows a significant directional variability inside the external field of view (FOV), an averaged spectrum representative for the FOV has to be constructed by weighting the radiance with the responsivity distribution over the FOV.
In general, in the case of an upward looking remote sensing spectrometer, the FOV convolution can be neglected and the spectrum irradiated along the instrumental line of sight is representative. In case of a limb sounding instrument strong vertical gradients in radiance arise especially at low tangent heights. The instrumental responsivity $R(\chi_1, \chi_2)$ to a point source in infinity as a function of its orientation with respect to the instrumental line of sight characterises the external field of view. The FOV is assumed to be small enough to project R onto a plane without significant distortion. χ_1, χ_2 are Cartesian coordinates measured in radians in this plane. The χ_1 axis is tangential to the vertical great circle containing the instrumental line of sight and the χ_2 axis is perpendicular to it and parallel to the horizon. The origin of the system coincides with the instrumental line of sight. The irradiated spectrum S

can be assumed to be independent from χ_2 and the averaged spectrum S_{av} is given by

$$\begin{aligned} S_{av} &= \int\int_{FOV} S(\chi_1) \times R(\chi_1, \chi_2) d\chi_1 d\chi_2 \\ &= \int_{\chi_1} S(\chi_1) \times \int_{\chi_2} R(\chi_1, \chi_2) d\chi_1 d\chi_2 \\ &= \int_{\chi_1} S(\chi_1) \times R_{vert}(\chi_1) d\chi_1 \end{aligned}$$

with

$$\int\int_{FOV} R(\chi_1, \chi_2) d\chi_1 d\chi_2 = 1 \quad \text{and} \quad R_{vert}(\chi_1) = \int_{\chi_2} R(\chi_1, \chi_2) d\chi_2$$

KOPRA subdivides the FOV in 20 horizontal bands of equal thickness. The user specifies the weight of each band $R_{vert,i}$ and the total vertical extent of the FOV H according to the characteristics of his instrument.

$$R_{vert,i} = \int_{\chi_1=\chi_i-\Delta\chi/2}^{\chi_i+\Delta\chi/2} R_{vert}(\chi_1) d\chi_1$$

with

$$\Delta\chi = 0.05 \times H \quad \text{and} \quad \chi_i = \Delta\chi \times (i - 10.5) \qquad i = 1, 2, 3, \cdots, 20$$

The irradiated spectrum has to be calculated for at least 3 relevant directions. Linear interpolation between adjacent calculated spectra yields $S_{interpol}(i)$ in the centre of band i. The averaged spectrum is approximated by KOPRA using

$$S_{av} \approx \frac{\sum_{i=1}^{20} R_{vert,i} \times S_{interpol}(i)}{\sum_{i=1}^{20} R_{vert,i}}$$

As can be seen, KOPRA does not demand $R_{vert} = 1$ for the weights of the bands in the input file. Any set of weights proportional to the normalised R_{vert} is valid also.

Since in a Fourier Transform spectrometer the optical path difference depends on the inclination of the wavefront in the interferometer, inhomogenous illumination of the FOV affects the spectral response also. This effect is of secondary importance. KOPRA allows to estimate the consequences on the measured spectrum assuming a circular internal FOV.

The relation between the optical path difference x and the inclination of the wavefront α versus optical axis *measured inside the interferometer* is

$$x(\alpha) = x(0) \times \cos(\alpha)$$

As a consequence, the contribution to the measured spectrum out of a cone surface centered on the optical axis has a common spectral shift versus the irradiated spectrum. A monochromatic line located at ν_0 is shifted to lower wavenumber $\nu(\alpha)$ in the measured spectrum. In small angle approximation one finds

$$\nu(\alpha) = \nu_0 \times (1 - 0.5 \times \alpha^2) \quad \text{and thus} \quad d\nu(\alpha) = -\nu_0 \times \alpha \times d\alpha$$

We consider an isotropic radiation field. The spectrum S contains a single monochromatic line with flux F_0

$$S(\nu) = F_0 \times \delta(\nu - \nu_0)$$

This line is mapped into a boxcar in the measured spectrum extending from $\nu_0 \times (1 - 0.5 \times \alpha_{max}^2)$ to ν_0. α_{max} is the maximal wavefront inclination accepted by the interferometer. The radiance (height of the boxcar) is $2F_0/\nu_0\alpha_{max}^2$. This is understandable in the following way: each distinct cone surface leads to a contribution proportional to its area $2\pi\alpha d\alpha$, that is smeared along the spectral abscissa over the interval $\nu_0\alpha d\alpha$. Both area and spectral width are proportional to α and so the radiances $\tilde{S}$ of all contributions are equal and a boxcar results.

$$\tilde{S}(\nu(\alpha)) = \frac{F_0}{\pi\alpha_{max}^2} \times \frac{2 \times \pi \times \alpha \times d\alpha}{\nu_0 \times \alpha \times d\alpha} = \frac{2 \times F_0}{\nu_0 \times \alpha_{max}^2}$$

The Fourier transform of the boxcar leads to the sinc-shaped self apodisation term (see section 'Calculation of AILS, self apodisation') in case of isotropic illumination. Next we consider an anisotropic radiation field. The spectrum S to consist of a single monochromatic line as before but the flux F depends on χ_1. We expand a Maclaurin series

$$\begin{aligned} S(\nu, \chi_1) &= F(\chi_1) \times \delta(\nu - \nu_0) \\ &= (F(0) + F' \times \chi_1 + 0.5 \times F'' \times \chi_1^2 + \cdots) \times \delta(\nu - \nu_0) \end{aligned}$$

To find the contribution of each cone surface, we have to integrate the flux in each concentric circle in the χ_1, χ_2 plane. We introduce the azimuthal coordinate ρ around the optical axis. The direction $\rho = 0$ is the positive χ_2 axis. The contribution of each cone surface is given by

$$\begin{aligned} \tilde{S}(\nu(\alpha)) &= \frac{1}{\pi \times \alpha_{max}^2} \times \frac{2}{\nu_0 \times \alpha} \\ &\quad \times \int_{\rho=-\pi/2}^{\pi/2} (F(0) + F' \times \chi_1 + 0.5 \times F'' \times \chi_1^2 + \cdots) \times \alpha \times d\rho \end{aligned}$$

The integration is performed by substituting the integration variable using $\alpha \times \sin(\rho) = \chi_1$. This leads to

$$\begin{aligned} \tilde{S}(\nu(\alpha)) &= \frac{1}{\pi \times \alpha_{max}^2} \times \frac{2}{\nu_0 \times \alpha} \\ &\quad \times \int_{\chi_1=-\alpha}^{\alpha} (F(0) + F' \times \chi_1 + 0.5 \times F'' \times \chi_1^2 + \cdots) \times \frac{1}{\sqrt{1 - \chi_1^2/\alpha^2}} d\chi_1 \end{aligned}$$

Due to the symmetry properties of the integrand all terms containing odd derivatives of F cancel. KOPRA omits derivatives higher than 2, therefore the error is of order O(4).

$$\tilde{S}(\nu(\alpha)) \approx \frac{1}{\pi \times \alpha_{max}^2} \times \frac{2}{\nu_0 \times \alpha} \times (\pi \times F(0) \times \alpha + 0.25 \times \pi \times F'' \times \alpha^3)$$

Substitution of α^2 using $\alpha^2 = 2 \times (1 - \nu/\nu_0)$ leads to

$$\tilde{S}(\nu(\alpha)) \approx \frac{2 \times F(0)}{\alpha_{max}^2 \times \nu_0} + \frac{F'' \times (1 - \nu/\nu_0)}{\alpha_{max}^2 \times \nu_0}$$

The additional second term describes a triangle of zero height at ν_0 and height $F''/2\nu_0$ at $\nu(\alpha_{max})$. The monochromatic line is mapped into a boxcar (connected to F(0)) with a slant increasing towards lower wavenumber (connected to F'') upon. An arbitrary spectrum can be interpreted as a dense superposition of monochromatic peaks. The relations given above for the monochromatic example therefore hold for the general case also.

To find $\tilde{S}$ for an arbitrary irradiated spectrum, KOPRA convolves S with a normalised boxcar extending along the spectral abscissa from $-0.25 \times \nu_0 \times \alpha_{max}^2$ to $+0.25 \times \nu_0 \times \alpha_{max}^2$. KOPRA calculates the second derivative of S with respect to the coordinate $\tilde{\chi_1} = \chi_1/\alpha_{max}$ fixing the maximal inclination in the interferometer as unit angle. $\delta^2 S/\delta\tilde{\chi_1}^2$ is convolved with a triangle. At $+0.25 \times \nu_0 \times \alpha_{max}^2$ the height of the triangle is zero. At $-0.25 \times \nu_0 \times \alpha_{max}^2$ the height of the triangle is a fourth of the boxcar height. Note that the bases of boxcar and triangle are centered on $\nu = 0$. KOPRA *does not perform any spectral scaling or shift on the calculated spectrum due to the finite FOV*. It is assumed that the spectral scaling due to finite FOV is absorbed in the spectral calibration of the instrument.
We expect the approximation to give more accurate results if the value for $\delta^2 S/\delta\tilde{\chi_1}^2$ is chosen appropriate for the extended FOV as a whole instead of using the value of $\delta^2 S/\delta\tilde{\chi_1}^2$ at $\tilde{\chi_1} = 0$. KOPRA constructs the representative value of the second derivative from three FOV-averaged spectra S_{av} to nominal and slightly up- and downward shifted line of sights.

7 Derivatives

In the retrieval process, derivatives with respect to all fitted parameters are needed. In the context under consideration here KOPRA offers derivatives with respect to elevation, spectral shift, ordinate offset, ordinate scale and parameters for AILS description.
We call the spectral distributions at the location of the instrument for specified LOS and FOV 'irradiated spectra' and the affiliated results of the measurements (without scale and offset consideration) 'instrumental spectra'. KOPRA models irradiated spectra and instrumental spectra yielding 'synthetic irradiated spectra' and 'synthetic instrumental spectra'. Scale and offset are considered via a multiplicative and additive constant, respectively, applied to the synthetic instrumental spectra: $S_{calcor} = aS_{instr} + b$. Spectra of the latter kind are used in the calculation of the derivatives.

- elevation

  The derivation with respect to elevation is calculated from the difference of two synthetic instrumental spectra, one referring to the specified line of sight, the other one to a slightly modified line of sight.
  If the FOV extent is neglected, KOPRA has only a single synthetic irradiated spectrum at its disposal. The complete forward calculation has to be repeated performing a renewed KOPRA run. If the FOV extent is taken into account, KOPRA has several synthetic irradiated spectra referring to different elevations at its disposal, and the two synthetic measured spectra needed are found by interpolation using the given set of synthetic irradiated spectra (see section 'field of view'). The increment in elevation is set to a small fraction (0.025) of the full vertical extent of the FOV.

- spectral shift

  The derivation with respect to spectral shift is calculated from the synthetic instrumental spectrum $S(i), i = 1, 2, \cdots, n_{max}$ by

  $$\frac{\delta S}{\delta \nu}(1) = \frac{S(2)-S(1)}{\Delta\nu}$$
  $$\frac{\delta S}{\delta \nu}(i) = \frac{S(i+1)-S(i-1)}{2\Delta\nu} \qquad 2 \le i \le n_{max} - 1$$
  $$\frac{\delta S}{\delta \nu}(n_{max}) = \frac{S(n_{max})-S(n_{max}-1)}{\Delta\nu}$$

- ordinate offset

The derivative of S_{calcor} with respect to an additional constant is unity.

- ordinate scale

  The derivative of S_{calcor} with respect to the multiplicative constant a is the synthetic instrumental spectrum S_{instr}.

- AILS parameters: modulation efficiency and phase error

  To calculate the derivative with respect to the modulation efficiency parameter m (see section 'Calculation of AILS') the AILS is calculated twice from the beginning. The derivative of the synthetic instrumental spectrum $S_{instr}(m_0)$ with respect to m is the convolution of the synthetic irradiated spectrum S_{irr} with the derivative of the AILS with respect to m.

$$\frac{\delta S_{instr}(m_0)}{\delta m} = \frac{AILS(m_0 + \Delta m) - AILS(m_0)}{\Delta m} \otimes S_{irr}$$

  The derivative with respect to phase error φ is calculated in the same way, but the amplitude of the modulation efficiency remains unchanged and is not recalculated. The increments used by KOPRA are $\Delta m = 10^{-3}$ and $\Delta\varphi = 10^{-4}$, well below the practical limit of retrieval accuracy.

- BOMEM AILS parameters: retroreflector linear shear variation along z-axis and IR misalignment along y direction

  The AILS is calculated twice from the beginning. The increments used by KOPRA are 10^{-4} in case of the linear shear variation along z-axis and 10^{-5} rad in case of IR misalignment, well below the practical limit of retrieval accuracy.