XGAUPROF

A GIPSY program to fit parameters of a Gauss function, the Gauss-Hermite series or a Voigt line-shape to data from GIPSY sets or ASCII files

May 7, 1999

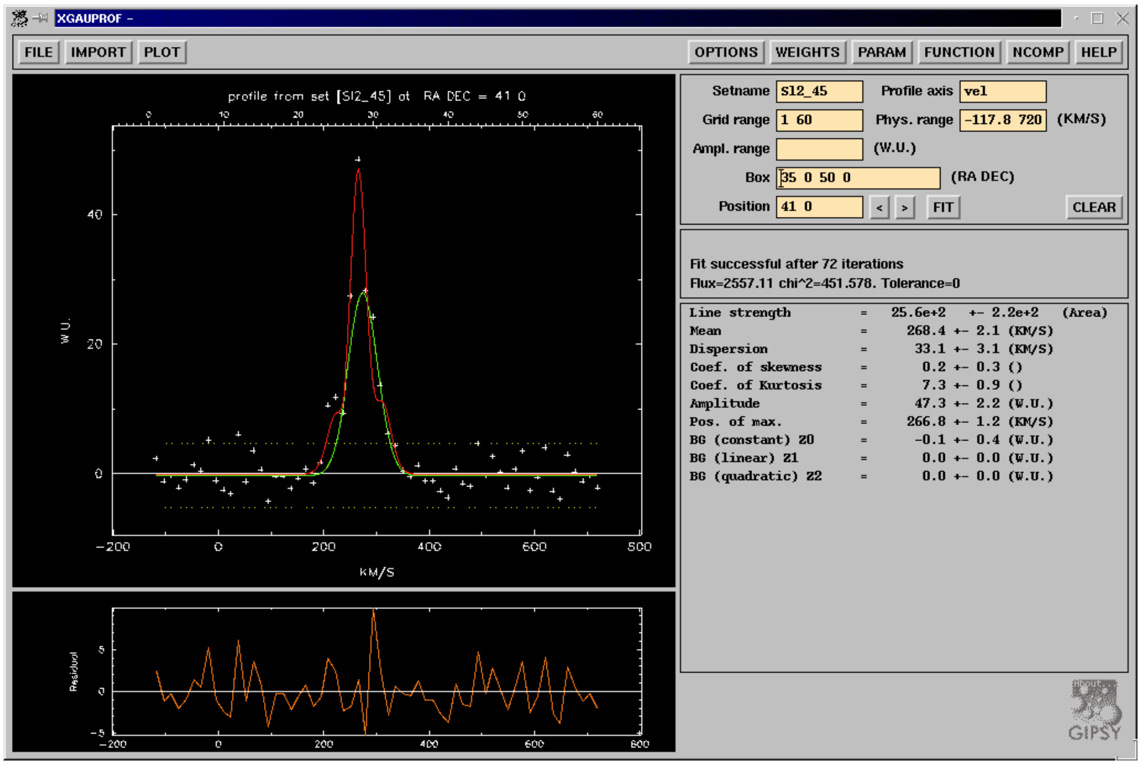

Figure 1: *XGAUPROF Graphical User Interface*

Chapter 1

Introduction

1.1 History

An article from 1966 called *Computer Analysis of Observed Distributions into Gaussian components* by Kaper et al. described a first Kapteyn Institute attempt to use a computer to decompose an observed frequency or intensity profile into a superposition of Gaussian components. A least squares method was applied to get a 'best fit' to study profiles of the spectral line at 21 cm. The program was implemented on a Stantec ZEBRA, installed in 1956. It had a memory of 8192 words of 33 bits. This limited the analysis to 150 data points and 6 parameters. The average access time to an address on the ZEBRA was 0.005 sec. and one least-squares iteration cycle took about 20 minutes. Initial guesses for the parameters were found by sketching a decomposition into Gaussians on a graph of the observed profile.

1.2 Standard Gauss

GIPSY program *XGAUPROF* finds best fit parameters for three functions given data from file or from a GIPSY set. The base function is a Gauss. The parameters are fitted with a least-squares fit algorithm which needs initial guesses. A special routine automates the procedure of getting reasonable estimates for a Gauss and the other functions in the program. The user can modify these values by hand using a graphical slider. A one component standard Gauss function with background is defined as:

$$\phi(x) = Ae^{-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2} + Z \tag{1.1}$$

Usually x is frequency or velocity. A is the amplitude at the center $x = x_0$ and σ is the dispersion of the profile, i.e. the half width at $\frac{A}{\sqrt{e}}$ and Z is a representation for the background.
In *XGAUPROF* the background consists of a constant, a linear and a quadratic term and is represented by:

$$Z = Z_0 + Z_1\,(x - x_0) + Z_2\,(x - x_0)^2 \tag{1.2}$$

The constant term Z_0 is often referred to as 'zero level'.

1.3 Gauss-Hermite series

If your profile deviates from a Gaussian shape (e.g. asymmetric profiles) then you can use the so called *Gauss-Hermite* series. The lowest order term of the series is a Gaussian. The higher order terms are orthogonal to this Gaussian. The higher order that we use in our fits are the parameters h_3 and h_4

measuring asymmetric and symmetric deviations of a Gaussian. The Gauss-Hermite function used in *XGAUPROF* is (Van der Marel & Franx):

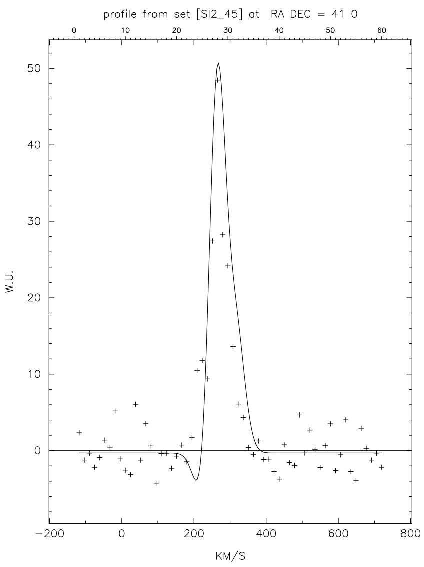

Figure 1.1: *Gauss-Hermite* $h3 = 0.2$, $h_4 = 0$.

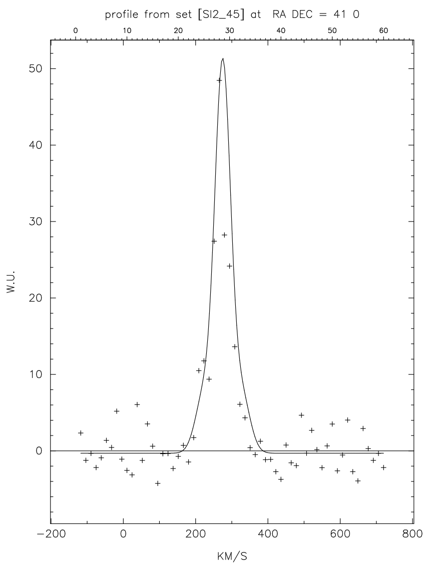

Figure 1.2: *Gauss-Hermite* $h3 = 0$, $h_4 = 0.1$.

$$\phi(x) = a\, e^{-\frac{1}{2}y^2} \left\{ 1 + \frac{h_3}{\sqrt{6}}(2\sqrt{2}y^3 - 3\sqrt{2}y) + \frac{h_4}{\sqrt{24}}(4y^4 - 12y^2 + 3) \right\} + Z \tag{1.3}$$

with $y \equiv \frac{x-b}{c}$. Note that the parameters a, b and c are equivalent to A, x_0 and σ of a Gaussian, only if $h_3 = h_4 = 0$.

1.4 Voigt profile

The line-shapes of spectroscopic transitions depend on the broadening mechanisms of the initial and final states, and include natural broadening, collisional broadening, power broadening, and Doppler broadening. Natural, collisional, and power broadening are homogeneous mechanisms and produce Lorentzian line-shapes. Doppler broadening is a form of inhomogeneous broadening and has a Gaussian line-shape. Combinations of Lorentzian and Gaussian line-shapes can be approximated by a Voigt profile. In fact, the Voigt profile is a convolution of these two line-shapes. It has the form:

$$\phi(\nu) = \frac{A}{\alpha_D}\sqrt{\frac{\ln(2)}{\pi}}\, K(x,y) + Z \tag{1.4}$$

$K(x, y)$ is the *Voigt function* and is defined as:

$$K(x,y) = \frac{y}{\pi}\int_{-\infty}^{\infty} \frac{e^{-t^2}}{y^2 + (x-t)^2} dt$$

where

$$y \equiv \frac{\alpha_L}{\alpha_D}\sqrt{\ln(2)} \quad \mathit{and} \quad x \equiv \frac{(\nu - \nu_0)}{\alpha_D}\sqrt{\ln(2)} \tag{1.5}$$

y is the ratio of Lorentz to Doppler widths and x the frequency scale (in units of the Doppler Line-shape half-width α_D.

Chapter 2

The standard Gauss function

2.1 Properties of a profile using moments of a distribution

One way to characterize a distribution is the use of its moments. The kth-*moment* of a distribution $\phi(x)$ is:

$$\mu_k = \int_{-\infty}^{\infty} (x - x_0)^k \, \phi(x) dx$$

With these moments one can calculate more familiar properties of a distribution like the line strength (i.e. area under the curve) γ, the mean X_0, the dispersion σ, the coefficient of skewness $\xi_1 \equiv \mu_3/\mu_2^{3/2}$ and the coefficient of kurtosis $\xi_2 \equiv \mu_4/\mu_2^2$. These quantities are calculated from:

$$\gamma \equiv \int_{-\infty}^{\infty} \phi(x)\, dx \qquad X_0 \equiv \frac{1}{\gamma} \int_{-\infty}^{\infty} x\, \phi(x)\, dx \qquad \sigma_0^2 \equiv \frac{1}{\gamma} \int_{-\infty}^{\infty} (x - X_0)^2 \, \phi(x)\, dx$$

$$\xi_i \equiv \frac{1}{\gamma} \int_{-\infty}^{\infty} \left((x - X_0)/\sigma\right)^{2+i} \, \phi(x)\, dx \qquad (i = 1, 2) \tag{2.1}$$

Skewness is a lack of symmetry in a distribution. If a distribution is symmetric about its mean it has zero skewness. The skewness defined above is called the Fisher Skewness.
Kurtosis is a measure of how "fat" the tails of a distribution are, measured relative to a normal distribution having the same standard deviation. A distribution is said to be *leptokurtic* if its tails are fatter than those of a corresponding normal distribution (high peak). It is said to be *platykurtic* if its tails are thinner than those of the normal distribution (flat-topped curve). The Fisher Kurtosis is defined by

$$\boxed{\xi_f = \xi_2 - 3} \tag{2.2}$$

From here we will use ξ_f if we talk about kurtosis.
Using the expressions above, one finds for our standard Gaussian:

The integrated line strength γ:

$$\gamma = \int_{-\infty}^{\infty} A e^{-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2} dx = A\,\sigma \sqrt{\frac{\pi}{2}}\, \mathrm{erf}\left(\frac{\mathrm{x} - \mathrm{x}_0}{\sigma\sqrt{2}}\right)\Big|_{-\infty}^{\infty}$$

erf is the 'error'-function and $\mathrm{erf}(-\infty) = -1$ and $\mathrm{erf}(\infty) = 1$.
Then:

$$\boxed{\gamma = A\sigma\sqrt{2\pi}} \tag{2.3}$$

The mean abscissa X_0:

$$\begin{aligned}
X_0 &= \frac{1}{\gamma}\int_{-\infty}^{\infty} x A e^{-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2} dx \\
&= \frac{1}{\gamma}\left[-A e^{-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2} + A\sqrt{\frac{\pi}{2}}\, x_0\, \sigma\, \mathrm{erf}\left(\frac{\mathrm{x}-\mathrm{x}_0}{\sigma\sqrt{2}}\right)\right]\Bigg|_{-\infty}^{\infty} \\
&= \frac{2}{\gamma} A\,\sigma\sqrt{\frac{\pi}{2}}\, x_0 = x_0
\end{aligned}$$

$$\boxed{X_0 = x_0} \tag{2.4}$$

The dispersion σ_0:

$$\begin{aligned}
\sigma_0^2 &= \frac{1}{\gamma}\int_{-\infty}^{\infty} (x-x_0)^2 A e^{-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2} dx \\
&= \frac{1}{\gamma}\left[-(x-x_0)\,\sigma^2\, A e^{-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2} + A\sqrt{\frac{\pi}{2}}\,\sigma^3\, \mathrm{erf}\left(\frac{\mathrm{x}-\mathrm{x}_0}{\sigma\sqrt{2}}\right)\right]\Bigg|_{-\infty}^{\infty} \\
&= \frac{2}{\gamma} A\sigma\sqrt{\frac{\pi}{2}}\,\sigma^2 = \sigma^2
\end{aligned}$$

$$\boxed{\sigma_0 = \sigma} \tag{2.5}$$

The Fisher coefficient of Skewness ξ_1:

$$\begin{aligned}
\xi_1 &= \frac{1}{\gamma}\int_{-\infty}^{\infty} \left(\frac{x-x_0}{\sigma}\right)^3 A e^{-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2} dx \\
&= \frac{1}{\gamma} A e^{-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2}\, \frac{-2\,(x-x_0)^2 - 4\,\sigma^2}{2\,\sigma}\Bigg|_{-\infty}^{\infty} \\
&= 0
\end{aligned}$$

$$\boxed{\xi_1 = 0} \tag{2.6}$$

This is what we expected for a symmetric distribution like a standard Gauss.

The Fisher coefficient of Kurtosis ξ_2:

$$\begin{aligned}
\xi_2 &= \frac{1}{\gamma}\int\limits_{-\infty}^{\infty}\left(\frac{x-x_0}{\sigma}\right)^4 A e^{\frac{-(x-x_0)^2}{2\sigma^2}}\,dx \\
&= \frac{1}{\gamma}\left[A\,e^{-\frac{(x-x_0)^2}{2\,\sigma^2}}\,\frac{-(x-x_0)^3-3\,(x-x_0)\,\sigma^2}{\sigma^2}+3\,A\sqrt{\frac{\pi}{2}}\,\sigma\,\mathrm{erf}\left(\frac{\mathrm{x}-\mathrm{x}_0}{\sqrt{2}\,\sigma}\right)\right]\Bigg|_{-\infty}^{\infty} \\
&= 3
\end{aligned}$$

$$\boxed{\xi_2 = 3} \tag{2.7}$$

$$\boxed{\xi_f = 0} \tag{2.8}$$

2.2 Partial derivatives of the standard Gauss function

The standard Gauss is represented by the formula:

$$\phi(x) = Ae^{-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2} + Z$$

The partial derivatives used in the least squares routine to fit the parameters are:

$$\frac{\partial\phi(x)}{\partial A} = e^{-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2} \tag{2.9}$$

$$\frac{\partial\phi(x)}{\partial x_0} = Ae^{-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2}\frac{(x-x_0)}{\sigma^2} \tag{2.10}$$

$$\frac{\partial\phi(x)}{\partial \sigma} = Ae^{-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2}\frac{(x-x_0)^2}{\sigma^3} \tag{2.11}$$

the derivatives for the background $Z = Z_0 + Z_1\,(x-x_0) + Z_2\,(x-x_0)^2$ are:

$$\frac{\partial\phi(x)}{\partial Z_0} = 1 \tag{2.12}$$

$$\frac{\partial\phi(x)}{\partial Z_1} = x - x_0 \tag{2.13}$$

$$\frac{\partial\phi(x)}{\partial Z_2} = (x-x_0)^2 \tag{2.14}$$

$$\tag{2.15}$$

2.3 Relation between FWHM and dispersion of a Gauss

Consider a standard Gauss function without any offset and symmetric around $x_0 = 0$:

$$f(x) = Ae^{-\frac{1}{2}\left(\frac{x}{\sigma}\right)^2}$$

To find a width at certain height given the dispersion, find a x_λ with $0 < \lambda < 1$ for which:

$$A\,e^{\frac{-x^2}{2\sigma^2}} = \lambda\,A \longrightarrow x_\lambda^2 = 2\sigma^2\ln\frac{1}{\lambda}$$

$$\boxed{x_\lambda = \sigma\sqrt{2Ln\tfrac{1}{\lambda}}}$$

A frequently used measure of profile width is the the Full Width at Half Maximum $fwhm$. This width can be expressed in σ by substitution of $\lambda = \frac{1}{2}$ and multiplication of the solution by 2 because the dispersion is a half width!

$$fwhm = 2\sigma\sqrt{2\ln\frac{1}{\frac{1}{2}}} = 2\sigma\sqrt{2\ln 2} \approx 2.355\,\sigma$$

$$\boxed{fwhm = 2\sigma\sqrt{2\ln 2}}$$

Note that the error in the fitted width at any height, increases or decreases with the same factor.

Chapter 3

The Gauss-Hermite series

The Gauss-Hermite (GH) series in *XGAUPROF* with $y \equiv \frac{x-b}{c}$ is represented by:

$$\phi(x) = a\, e^{-\frac{1}{2}y^2} \left\{ 1 + \frac{h_3}{\sqrt{6}}(2\sqrt{2}y^3 - 3\sqrt{2}y) + \frac{h_4}{\sqrt{24}}(4y^4 - 12y^2 + 3) \right\} + Z$$

Simplify this equation further:

$$\phi(x) = a\, E\, \left\{ 1 + h_3(c_1 y + c_3 y^3) + h_4(c_0 + c_2 y^2 + c_4 y^4) \right\}$$

or:

$$\phi(x) = a\, E\, Q$$

with $E \equiv e^{-\frac{1}{2}y^2}$, $Q = \left\{ 1 + h_3(c_1 y + c_3 y^3) + h_4(c_0 + c_2 y^2 + c_4 y^4) \right\}$ and further:

$$c_0 = \frac{1}{4}\sqrt{6} \quad c_1 = -\sqrt{3} \quad c_2 = -\sqrt{6} \quad c_3 = \frac{2}{3}\sqrt{3} \quad c_4 = \frac{1}{3}\sqrt{6}$$

Then the partial derivatives used in the least-squares fit routine are:

$$\frac{\partial\phi(x)}{\partial a} = E\, Q \tag{3.1}$$

$$\frac{\partial\phi(x)}{\partial b} = a\, E\, \frac{1}{c}\left[h_3(-c_1 - 3c_3 y^2) + h_4(-2c_2 y - 4c_4 y^3) + y\, Q \right] \tag{3.2}$$

$$\frac{\partial\phi(x)}{\partial c} = a\, E\, \frac{1}{c}\left[h_3(-c_1 y - 3c_3 y^3) + h_4(-2c_2 y^2 - 4c_4 y^4) + y^2\, Q \right] = y\, \frac{\partial\phi(x)}{\partial b} \tag{3.3}$$

$$\frac{\partial\phi(x)}{\partial h_3} = a\, E\, (c_1 y + c_3 y^3) \tag{3.4}$$

$$\frac{\partial\phi(x)}{\partial h_4} = a\, E\, (c_0 + c_2 y^2 + c_4 y^4) \tag{3.5}$$

Note that $\frac{\partial\phi(x)}{\partial x} = -\frac{\partial\phi(x)}{\partial b}$. We will need this expression if we want to calculate the position of the maximum of the GH series. This position is only equal to parameter b if $h_3 = h_4 = 0$! To find the real maximum, solve:

$$\frac{\partial\phi(x)}{\partial x} = -a\, E\, \frac{1}{c}\left[h_3(-c_1 - 3c_3 y^2) + h_4(-2c_2 y - 4c_4 y^3) + y\, Q \right] = 0$$

which means solving:

$$h_3(-c_1 - 3c_3 y^2) + h_4(-2c_2 y - 4c_4 y^3) + y\, \left\{ 1 + h_3(c_1 y + c_3 y^3) + h_4(c_0 + c_2 y^2 + c_4 y^4) \right\} = 0$$

After rearranging the equation above we get:

$$\lambda_5 y^5 + \lambda_4 y^4 + \lambda_3 y^3 + \lambda_2 y^2 + \lambda_1 y + \lambda_0 = 0 \tag{3.6}$$

with coefficients equal to:

$$\begin{aligned}
\lambda_0 &= -h_3\, c_1 \\
\lambda_1 &= h_4\,(c_0 - 2c_2) + 1 \\
\lambda_2 &= h_3\,(c_1 - 3c_3) \\
\lambda_3 &= h_4\,(c_2 - 4c_4) \\
\lambda_4 &= h_3\, c_3 \\
\lambda_5 &= h_4\, c_4
\end{aligned}$$

We applied a bisection to solve the equation. For initial limits we use $x_1 = b - \frac{1}{2}c$ and $x_2 = b + \frac{1}{2}c$ which for the bisection equation is the same as $y_1 = -\frac{1}{2}$ and $y_2 = \frac{1}{2}$.

3.1 Moments of the GH series

As stated before, in the function:

$$\phi(x) = a\, e^{-\frac{1}{2}y^2},\left\{1 + h_3(c_1 y + c_3 y^3) + h_4(c_0 + c_2 y^2 + c_4 y^4)\right\}$$

with:

$$y \equiv \frac{x-b}{c}$$

the parameters a, b and c are only equal to A, x_0 and σ of a standard Gaussian, if $h_3 = h_4 = 0$. If we want to compare these parameters for h_3 and/or h_4 unequal to 0 then we have to calculate the profile properties using the moments of the GH distribution:

The integrated line strength γ:

$$\gamma = \int_{-\infty}^{\infty} \phi(x)dx = a\,c\,\sqrt{2\pi}\,(1 + c_0\, h_4 + c_2\, h_4 + 3c_4\, h_4) = a\,c\,\sqrt{2\pi}(1 + \frac{1}{4}\sqrt{6}\, h_4)$$

$$\boxed{\gamma = a\,c\,\sqrt{2\pi}(1 + \tfrac{1}{4}\sqrt{6}\, h_4)} \tag{3.7}$$

The mean abscissa X_0:

$$\begin{aligned}
X_0 &= \frac{1}{\gamma}\int_{-\infty}^{\infty} x\phi(x)dx \\
&= \frac{1}{\gamma} a\,c\,\sqrt{2\pi}\;(b + c\,c_1\, h_3 + 3c\,c_3\, h_3 + b\,c_0\, h_4 + b\,c_2\, h_4 + 3b\,c_4\, h_4) \\
&= \frac{1}{\gamma} a\,c\,\sqrt{2\pi}\left[b\,(1 + \frac{1}{4}\sqrt{6}\, h_4) + c\,(\sqrt{3}\, h_3)\right] \\
&= b + c\,\frac{\sqrt{3}\, h_3}{1 + \frac{1}{4}\sqrt{6}\, h_4} \\
&\approx b + c\,\left[\sqrt{3}\, h_3\,(1 - \frac{1}{4}\sqrt{6}\, h_4)\right]
\end{aligned}$$

The last step is an approximation. Remember that $(1+\alpha\, x)^{\beta} \approx 1-\alpha\,\beta\, x$ for small x. If we include only the lowest order terms in h_3 and h_4, then:

$$\boxed{X_0 \approx b + \sqrt{3}\, h_3\, c} \tag{3.8}$$

The dispersion σ_0:

$$\begin{aligned}
\sigma_0^2 &= \frac{1}{\gamma} \int\limits_{-\infty}^{\infty} (x - X_0)^2 \phi(x) dx \\
&\approx \frac{1}{\gamma}\, a\, c\, \sqrt{2\pi}\, c^2\, \frac{(1 + 3c_0\, h_4 + 5c_2\, h_4 + 21c_4\, h4)}{(1 + c_0\, h_4 + c_2\, h_4 + 3c_4\, h_4)^2} \\
&= c^2\, \frac{(1 + 3c_0\, h_4 + 5c_2\, h_4 + 21c_4\, h4)}{(1 + c_0\, h_4 + c_2\, h_4 + 3c_4\, h_4)^3} \\
&= c^2\, \frac{1 + 2\frac{3}{4}\sqrt{6}\, h_4}{\left(1 + \frac{1}{4}\sqrt{6}\, h_4\right)^3} \\
&\approx c^2\, (1 + 2\sqrt{6}\, h_4)
\end{aligned}$$

$$\boxed{\sigma_0 \approx c\sqrt{1 + 2\sqrt{6}\, h_4} \approx c\, (1 + \sqrt{6}\, h_4)} \tag{3.9}$$

The Fisher coefficient of Skewness ξ_1:
A set of observations that is not symmetrically distributed is said to be skewed. If the distribution has a longer tail less than the maximum, the function has *negative skewness.* Otherwise, it has *positive skewness.*

$$\begin{aligned}
\xi_1 &= \frac{1}{\gamma} \int\limits_{-\infty}^{\infty} \left(\frac{x - x_0}{\sigma}\right)^3 \phi(x) dx \\
&\approx \frac{1}{\gamma}\, \frac{2a\, c\, \sqrt{2\pi}\, c^3\, 3\, c_3 h_3}{(1 + c_0\, h_4 + c_2\, h_4 + 3c_4\, h_4)^3 \left(\frac{c^2 (1 + h_4\, (3c_0 + 5c_2 + 21c_4))}{(1 + c_0\, h_4 + c_2\, h_4 + 3c_4\, h_4)^3}\right)^{\frac{3}{2}}} \\
&= \frac{6\, c_3\, h_3\, (1 + c_0\, h_4 + c_2\, h_4 + 3c_4\, h_4)^{\frac{1}{2}}}{(1 + h_4\, (3c_0 + 5c_2 + 21c_4))^{\frac{3}{2}}} \\
&= \frac{4\sqrt{3}\, h_3\, (1 + \frac{1}{4}\sqrt{6}\, h_4)^{\frac{1}{2}}}{\left(1 + 2\frac{3}{4}\sqrt{6}\, h_4\right)^{\frac{3}{2}}}
\end{aligned}$$

$$\boxed{\xi_1 \approx 4\sqrt{3}\, h_3} \tag{3.10}$$

This is what we could have expected because h_3 is the parameter that measures asymmetric deviations.

The Fisher coefficient of Kurtosis ξ_2:

$$\begin{aligned}
\xi_2 &= \frac{1}{\gamma}\int_{-\infty}^{\infty}\left(\frac{x-X_0}{\sigma}\right)^4 \phi(x)dx \\
&\approx \frac{1}{\gamma}\,\frac{-3ac\sqrt{2\pi}\,(1+c_0h_4+c_2h_4+3c_4h_4)^2\,(-1-5c_0h_4-9c_2h_4-47c_4h_4)}{(1+3c_0h_4+5c_2h_4+21c_4h_4)^2} \\
&= \frac{3\,(1+h_4\,(c_0+c_2+3c_4)(1+h_4\,(5c_0+9c_2+47c_4)}{(1+h_4\,(3c_0+5c_2+21c_4))^2} \\
&= \frac{3(1+\frac{1}{4}\sqrt{6}\,h_4)(1+\frac{95}{12}\sqrt{6}\,h_4)}{\left(1+2\frac{3}{4}\sqrt{6}\,h_4\right)^2}
\end{aligned}$$

$$\boxed{\xi_2 \approx 3+8\sqrt{6}\,h_4} \tag{3.11}$$

$$\boxed{\xi_f \approx 8\sqrt{6}\,h_4} \tag{3.12}$$

The initial guesses for the h_3 and h_4 parameters in the least-squares fit, are set to zero because we expect that the profile will still resemble the standard Gaussian. If a fit is successful, the profile parameters γ, X_0 and σ, skewness and kurtosis are calculated from a,b, c, h_3 and h_4 using the formulas above. For the errors in these parameters we derived:

$$\Delta\gamma = \frac{1}{\gamma}\sqrt{\left(\frac{\Delta a}{a}\right)^2+\left(\frac{\Delta c}{c}\right)^2+\left(\frac{1}{\frac{2}{3}\sqrt{6}+h_4}\right)^2\left(\frac{\Delta h_4}{h_4}\right)^2} \tag{3.13}$$

$$\Delta X_0 = \sqrt{(\Delta b)^2+3h_3^2(\Delta c)^2+3c^2(\Delta h_3)^2} \tag{3.14}$$

$$\Delta\sigma_0 = \sqrt{\left(1+\sqrt{6}\,h_4\right)^2(\Delta c)^2+6c^2(\Delta h_4)^2} \tag{3.15}$$

$$\Delta\xi_1 = 4\sqrt{3}\,\Delta h_3 \tag{3.16}$$

$$\Delta\xi_2 = 8\sqrt{6}\,\Delta h_4 \tag{3.17}$$

Chapter 4

The Voigt profile

The Voigt profile is a line-shape which results form a convolution of Lorentzian and Doppler line broadening mechanisms:

$$\phi_{Lorentz}(\nu) = \frac{1}{\pi}\frac{\alpha_L}{(\nu-\nu_0)^2+\alpha_L^2} \tag{4.1}$$

$$\phi_{Doppler}(\nu) = \frac{1}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}}e^{-\ln 2\frac{(\nu-\nu_0)^2}{\alpha_D^2}} \tag{4.2}$$

Both functions are normalized. α_D **and** α_L **are half widths at half maximum**. Convolution is given by the relation

$$f(\nu)\star g(\nu) = \int_{-\infty}^{\infty} f(\nu-t)g(t)dt$$

Define the ratio of Lorentz to Doppler widths as

$$y \equiv \frac{\alpha_L}{\alpha_D}\sqrt{\ln 2} \tag{4.3}$$

and the frequency scale (in units of the Doppler Line-shape half-width α_D)

$$x \equiv \frac{\nu-\nu_0}{\alpha_D}\sqrt{\ln 2} \tag{4.4}$$

then:

$$\phi_L(\nu) = \frac{1}{\pi}\frac{\sqrt{\ln 2}}{\alpha_D}\frac{y}{x^2+y^2}$$

and

$$\phi_D(\nu) = \frac{1}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}}e^{-x^2}$$

The convolution:

$$\phi_L(\nu)\star\phi_D(\nu) = \int_{-\infty}^{\infty}\frac{1}{\pi}\frac{\sqrt{\ln 2}}{\alpha_D}\frac{y}{(x-t')^2+y^2}\frac{1}{\alpha_D}\frac{\sqrt{\ln 2}}{\sqrt{\pi}}e^{-t'^2}dt$$

If you replace ν by $\nu - t$ in the expression for x, then

$$x - t' = \frac{\nu - t}{\alpha_D}\sqrt{\ln 2} - \frac{\nu_0}{\alpha_D}\sqrt{\ln 2} = \frac{\nu-\nu_0}{\alpha_D}\sqrt{\ln 2} - t\frac{\sqrt{\ln 2}}{\alpha_D} = x - \frac{\sqrt{\ln 2}}{\alpha_D}t$$

and we conclude that $t' = \frac{\sqrt{\ln 2}}{\alpha_D} t$ and $dt' = \frac{\sqrt{\ln 2}}{\alpha_D} dt \Leftrightarrow dt = \frac{\alpha_D}{\sqrt{\ln 2}} dt'$

$$\phi_L(\nu) \star \phi_D(\nu) = \frac{1}{\alpha_D} \frac{\sqrt{\ln 2}}{\alpha_D} \frac{\sqrt{\ln 2}}{\sqrt{\pi}} \frac{\alpha_D}{\sqrt{\ln 2}} \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t'^2}}{(x-t')^2 + y^2} dt'$$

Replace t' by t to obtain:

$$\phi_\nu(\nu) = \phi_L(\nu) \star \phi_D(\nu) = \frac{1}{\alpha_D} \sqrt{\frac{\ln 2}{\pi}} \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{(x-t)^2 + y^2} dt \tag{4.5}$$

As we will see in the next section: $\int_{-\infty}^{\infty} \phi_\nu(\nu) d\nu = 1$ so the Voigt profile (eq.4.5) is also normalized.

4.1 The Voigt function $K(x, y)$

Part of the expression for the Voigt line-shape is the Voigt function. The formula for this function is:

$$K(x, y) = \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{y^2 + (x-t)^2} dt$$

Consider:

$$\int_0^{\infty} e^{-yv} \cos\left((x-t)v\right) dv = \frac{y}{(x-t)^2 + y^2} \rightarrow$$

$$\begin{aligned}
K(x, y) &= \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{y e^{-t^2}}{(x-t)^2 + y^2} \, dt \\
&= \frac{1}{\pi} \int_{-\infty}^{+\infty} e^{-t^2} \int_0^{\infty} e^{-yv} \cos\left((x-t)v\right) dv \, dt \\
&= \frac{1}{\pi} \int_0^{\infty} e^{-yv} \int_{-\infty}^{+\infty} e^{-t^2} \cos\left((x-t)v\right) dt \, dv \\
&= \frac{1}{\pi} \int_0^{\infty} e^{-yv} \cos yv \int_{-\infty}^{+\infty} e^{-t^2} \cos tv \, dt \, dv
\end{aligned}$$

Consider:

$$\int_{-\infty}^{+\infty} e^{-t^2} \cos(tv) dt = \sqrt{\pi} e^{-\frac{v^2}{4}} \rightarrow$$

$$\begin{aligned} K(x,y) &= \frac{1}{\sqrt{\pi}} \int_0^\infty e^{-\frac{v^2}{4}} e^{-yv} \cos(tv)\, dv \\ &= \frac{1}{2\sqrt{\pi}} \int_0^\infty e^{-\frac{v^2}{4}-yv} (e^{itv} + e^{-itv}) dv \\ &= \frac{1}{2\sqrt{\pi}} \int_0^\infty (e^{-\frac{v^2}{4}-(y-it)v} + e^{-\frac{v^2}{4}-(y+it)v}) dv \end{aligned}$$

Let $z = t + iy$, then $iz = -(y - it)$, $\mathrm{i}\overline{z} = (y + it)$

$$K(x,y) = \frac{1}{2\sqrt{\pi}} \int_0^\infty (e^{-(\frac{v}{2}-iz)^2 - z^2} + e^{-(\frac{v}{2}+i\overline{z})^2 - \overline{z}^2}) dv$$

Let $u1 = v/2 - iz$ and $u_2 = v/2 + iz$

$$K(x,y) = \frac{1}{\sqrt{\pi}}\, e^{-z^2} \int_{-iz}^\infty e^{-{u_1}^2} du_1 \; + \; \frac{e^{-\bar{z}^2}}{\sqrt{\pi}} \int_{i\bar{z}}^\infty e^{-{u_2}^2} du_2$$

According to Abramowitz & Stegun (AS): $\mathrm{erfc(z)} \equiv \frac{2}{\sqrt{\pi}} \int_{\mathrm{z}}^\infty \mathrm{e}^{-\mathrm{t}^2} \mathrm{dt}$ so that:

$$K(x,y) = \frac{1}{2} \left(e^{-z^2} \mathrm{erfc(-iz)} \; + \mathrm{e}^{-\bar{\mathrm{z}}^2} \mathrm{erfc(i\bar{z})}\right) \tag{4.6}$$

In AS we find the function $\omega(z)$ defined as:

$$\omega(z) = e^{-z^2} \mathrm{erfc(-iz)} \tag{4.7}$$

With the relations above one recognizes the relation $\omega(\bar{z}) = \overline{\omega(-z)}$. If we write the Voigt function in terms of function w then:

$$K(x,y) = \frac{1}{2}\{\omega(z) + \omega(-\bar{z})\} = \frac{1}{2}\{\omega(z) + \overline{\omega(z)}\} = \Re\{\omega(z)\}$$

$$\boxed{K(x,y) = \Re\{\omega(z)\}} \tag{4.8}$$

4.2 Area under the Voigt Line-shape

Remember the Voigt line-shape was given by:

$$\phi(\nu) = \frac{A}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}}\frac{y}{\pi}\int_{t=-\infty}^{t=\infty}\frac{e^{-t^2}}{y^2+(x-t)^2}dt \tag{4.9}$$

We want to evaluate $\int_{-\infty}^{\infty}\phi(\nu)d\nu$. By changing the integration order, one can write:

$$\int_{\nu=-\infty}^{\nu=\infty}\phi(\nu)d\nu = \frac{A}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}}\int_{t=-\infty}^{t=\infty}\frac{y}{\pi}\left\{\int_{\nu=-\infty}^{\nu=\infty}\frac{e^{-t^2}}{y^2+(x-t)^2}d\nu\right\}dt$$

Because $x \equiv \frac{\nu-\nu_0}{\alpha_D}\sqrt{\ln 2}$, we derive $d\nu = \frac{\alpha_D}{\sqrt{\ln 2}}dx$

$$\int_{-\infty}^{\infty}\phi(\nu)d\nu = \frac{A}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}}\frac{\alpha_D}{\sqrt{\ln 2}}\int_{-\infty}^{\infty}\frac{y}{\pi}\left\{\int_{-\infty}^{\infty}\frac{e^{-t^2}}{y^2+(x-t)^2}dx\right\}dt$$

The inner integral $\int_{-\infty}^{\infty}\frac{1}{y^2+(x-t)^2}dx = \frac{1}{y}\arctan\left(\frac{x-t}{y}\right)\Big|_{-\infty}^{\infty} = \frac{\pi}{y}$ so that:

$$\int_{-\infty}^{\infty}\phi(\nu)d\nu = \frac{A}{\sqrt{\pi}}\int_{-\infty}^{\infty}e^{-t^2}dt = \frac{A}{\sqrt{\pi}}\cdot\sqrt{\pi} = A$$

This proves what we already expected. Besides the area scaling factor A (which is a fit parameter in the least-squares fit) the area of the convolution of the two functions (Lorentzian and Doppler line-shapes) is normalized. The amplitude is found at $\nu = \nu_0$. Then according to its definition $x = 0$ and the relation between the amplitude and area is $amp = \phi(\nu_0)$:

$$\boxed{amp = \frac{A}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}}K(0,y)} \tag{4.10}$$

The error in the amplitude is then:

$$\begin{aligned}\Delta amp &= \sqrt{\frac{\ln 2}{\pi}}K(0,y)\sqrt{\left(\frac{\partial}{\partial\alpha_D}\frac{A}{\alpha_D}\Delta\alpha_D\right)^2+\left(\frac{\partial}{\partial A}\frac{A}{\alpha_D}\Delta A\right)^2}\\ &= \sqrt{\frac{\ln 2}{\pi}}K(0,y)\sqrt{\left(\frac{A}{\alpha_D^2}\Delta\alpha_D^2\right)^2+\left(\frac{1}{\alpha_D^2}\Delta A\right)^2}\end{aligned}$$

$$\boxed{\Delta amp = amp\sqrt{\left(\frac{\Delta\alpha_D}{\alpha_D}\right)^2+\left(\frac{\Delta A}{A}\right)^2}} \tag{4.11}$$

4.3 Partial derivatives of the Voigt Function

Consider the relations $z = x + iy$ and $-\bar{z} = -x + iy$. Then:

$$\frac{\partial\omega}{\partial x} = \frac{\partial z}{\partial x}\frac{\partial\omega}{\partial z} = \frac{\partial(x+iy)}{\partial x}\frac{\partial\omega}{\partial z} = \frac{\partial\omega}{\partial z}$$

$$\frac{\partial\omega}{\partial x} = \frac{\partial(-\bar{z})}{\partial x}\frac{\partial\omega}{\partial(-\bar{z})} = \frac{\partial(-x+iy)}{\partial x}\frac{\partial\omega}{\partial(-\bar{z})} = \frac{-\partial\omega}{\partial(-\bar{z})}$$

$$\frac{\partial\omega}{\partial y} = \frac{\partial z}{\partial y}\frac{\partial\omega}{\partial z} = \frac{\partial(x+iy)}{\partial y}\frac{\partial\omega}{\partial z} = i\frac{\partial\omega}{\partial z}$$

$$\frac{\partial\omega}{\partial y} = \frac{\partial(-\bar{z})}{\partial y}\frac{\partial\omega}{\partial(-\bar{z})} = \frac{\partial(-x+iy)}{\partial y}\frac{\partial\omega}{\partial(-\bar{z})} = i\frac{-\partial\omega}{\partial(-\bar{z})}$$

Now it is necessary to find $\frac{\partial\omega(z)}{\partial z}$. In Abramowitz & Stegun we find the relation $\frac{\partial\omega(z)}{\partial z} = -2z\omega(z) + \frac{2i}{\sqrt{\pi}}$. Then:

$$\begin{aligned}
\frac{\partial K(x,y)}{\partial x} &= \frac{\partial}{\partial x}\left\{\frac{1}{2}\left(\omega(z)+\omega(-\bar{z})\right)\right\} \\
&= \frac{1}{2}\left\{\frac{\partial\omega(z)}{\partial x} + \frac{\partial\omega(-\bar{z})}{\partial x}\right\} \\
&= \frac{1}{2}\left\{\frac{\partial}{\partial z}\omega(z) - \frac{\partial}{\partial(-\bar{z})}\omega(-\bar{z})\right\} \\
&= \frac{1}{2}\left\{-2z\omega(z) + \frac{2i}{\sqrt{\pi}} - \left(-2(-\bar{z})\omega(-\bar{z}) + \frac{2i}{\sqrt{\pi}}\right)\right\} \\
&= -\left(z\omega(z) + \bar{z}\omega(-\bar{z})\right)
\end{aligned}$$

with $\omega(-\bar{z}) = \overline{\omega(z)}$:

$$\begin{aligned}
&= -\left(z\omega(z) + \overline{z\omega(z)}\right) \\
&= -2\Re\left\{z\omega(z)\right\}
\end{aligned}$$

In the same way we write:

$$\begin{aligned}
\frac{\partial K(x,y)}{\partial y} &= \frac{\partial}{\partial y}\left\{\frac{1}{2}\left(\omega(z)+\omega(-\bar{z})\right)\right\} \\
&= \frac{1}{2}\left\{\frac{\partial\omega(z)}{\partial y} + \frac{\partial\omega(-\bar{z})}{\partial y}\right\} \\
&= \frac{i}{2}\left\{\frac{\partial\omega(z)}{\partial z} + i\frac{\partial\omega(-\overline{z})}{\partial(-\overline{z})}\right\} \\
&= \frac{i}{2}\left\{-2z\omega(z) + \frac{2i}{\sqrt{\pi}} + -z(-\overline{z})\omega(-\overline{z}) + \frac{2i}{\sqrt{\pi}}\right\} \\
&= -\frac{2}{\sqrt{\pi}} - i\left\{z\omega(z) - \overline{z}\omega(-\overline{z})\right\} \\
&= -\frac{2}{\sqrt{\pi}} - i\{z\omega(z) - \overline{z\omega(z)}\} \qquad (\textit{because } \omega(-\overline{z}) = \overline{\omega(z)}) \\
&= -\frac{2}{\sqrt{\pi}} + 2\Im\{z\omega(z)\}
\end{aligned}$$

To summarize:

$$\boxed{\frac{\partial K(x,y)}{\partial y} = -2\Re\{z\omega(z)\}} \tag{4.12}$$

$$\boxed{\frac{\partial k(x,y)}{\partial y} = -\frac{2}{\sqrt{\pi}} + 2\Im\{z\omega(z)\}} \tag{4.13}$$

4.4 Partial derivatives of the Voigt Line-shape

Lets start to recall some definitions:

$$\phi(v) = \frac{A}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}} K(x,y) \qquad K(x,y) = \Re\{\omega(z)\}$$

with:

$$x = \frac{v - v_0}{\alpha_D}\sqrt{\ln 2} \qquad y = \frac{\alpha_L}{\alpha_D}\sqrt{\ln 2}$$

$$\frac{\partial}{\partial x} K(x,y) = -2\Re\{z\omega(z)\}, \quad \frac{\partial}{\partial y} K(x,y) = -\frac{2}{\sqrt{\pi}} + 2\Im\{z\omega(z)\}$$

Then:

$$\frac{\partial \phi}{\partial A} = \frac{1}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}} K(x,y) = \frac{1}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}} \Re\{\omega(z)\} \tag{4.14}$$

$$\frac{\partial \phi}{\partial v_0} = \frac{A}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}} \frac{\partial}{\partial x} K(x,y) \frac{\partial x}{\partial v} = \frac{A}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}} \left\{-2\Re\{z\omega(z)\}\right\} \frac{-1}{\alpha_D}\sqrt{\ln 2} \tag{4.15}$$

$$\frac{\partial \phi}{\partial \alpha_L} = \frac{A}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}} \frac{\partial}{\partial y} K(x,y) \frac{\partial y}{\partial v} = \frac{A}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}} \left\{-\frac{2}{\sqrt{\pi}} + 2\Im\{z\omega(z)\}\right\} \frac{1}{\alpha_D}\sqrt{\ln 2} \tag{4.16}$$

$$\begin{aligned}
\frac{\partial \phi}{\partial \alpha_D} &= K(x,y) \frac{\partial}{\partial \alpha_D}\left\{\frac{A}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}}\right\} + \frac{A}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}} \frac{\partial}{\partial \alpha_D} K(x,y) \\
&= A\sqrt{\frac{\ln 2}{\pi}} \left(-\frac{K(x,y)}{\alpha_D^2} + \frac{1}{\alpha_D}\left\{\frac{\partial}{\partial x} K(x,y) \frac{\partial}{\partial \alpha_D}\left[\frac{v - v_0}{\alpha_D}\sqrt{\ln 2}\right] + \frac{\partial}{\partial y} K(x,y) \frac{\partial}{\partial \alpha_D}\left[\frac{\alpha_L}{\alpha_D}\sqrt{\ln 2}\right]\right\}\right) \\
&= A\sqrt{\frac{\ln 2}{\pi}} \left(-\frac{K(x,y)}{\alpha_D^2} + \frac{1}{\alpha_D}\left\{-\frac{v - v_0}{\alpha_D^2}\sqrt{\ln 2}\frac{\partial}{\partial x} K(x,y) - \frac{\alpha_L}{\alpha_D^2}\sqrt{\ln 2}\frac{\partial}{\partial y} K(x,y)\right\}\right) \\
&= \frac{A}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}} \frac{1}{\alpha_D}\left(-K(x,y) + \left\{-x\frac{\partial}{\partial x} K(x,y) - y\frac{\partial}{\partial y} K(x,y)\right\}\right) \\
&= -\frac{A}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}} \frac{1}{\alpha_D}\left(K(x,y) + x\frac{\partial}{\partial x} K(x,y) + y\frac{\partial}{\partial y} K(x,y)\right)
\end{aligned} \tag{4.17}$$

Chapter 5

Initial estimates

We automated calculating initial estimates using a method described by Schwarz (1968) called the *gauest* method. A second-order polynomial is fitted at each pixel position x_k using $2Q + 1$ points distributed symmetrically around x_k. The value at x_k is *not* the profile value at that point, but the median of that value and the two neighbours. Outliers that are not filtered with this median filter can be masked in the plot with the left mouse button. In $XGAUPROF$ the factor Q is called the smoothing factor. The coefficient of the second-order term of the polynomial is an approximation of the second derivative of the observed profile. Assuming that the observed profile can be approximated by the sum of a few (standard) Gaussian functions, the parameters x_0 and σ_0 are calculated from the main minima of the second derivative. The amplitude is derived from the observed profile. Tests using different threshold values make it possible to discriminate against spurious components; the threshold values depend on Q and the r.m.s. noise of the observed profile. The Gaussian components are then subtracted from the observed profile, and the residual profile, mainly the sum of a few remaining broader components, is handled in the same way as the original. Profiles with a maximum amplitude smaller than a user given value and profiles with a dispersion smaller than a user given value are discarded. The initial values for these filters are set to zero. Blanks in the profile and points that are masked by the user are set to the value of the zero level. If you did not fix a certain zero level, then the median of the profile is used as an estimate. If you did not fix the r.m.s. noise of the observed profile, the distance between the quartiles of the profile is used as an estimate.

Chapter 6

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