1

About Voigt Profile

1.1. Definition

In spectroscopy, it is usually needed to broaden specific peak profile. The broadening mechnism is then usually through convolution with the predefined broadening function. Here Voigt profile is one of the commonly used profiles. Basically, it is obtained by simply convoluting the Gaussian normal distribution profile (or Google it, which will lead to corresponding Wikipage) with the Lorentzian profile . (or Google it, which will lead to corresponding Wikipage). First of all, it is given the standard form of the above two commonly used probability distribution function (PDF, usually given as lower case 'f', in contrast to the cumulative distribution function, which is usually given as upper case 'F'). To distingush between Gaussian and Lorentzian profile in this context, the symbol 'g' was assigned for the PDF of Gaussian profile and 'l' for Lorentzian profile.

1.1.1. Gaussian Profile

$$g[x\_] := \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \text{ (*General form, given as the commonly used mathematical form.*)}$$

```
g[x_] := (Exp[-x^2 / (2 σ^2)]) / (σ Sqrt[2 π])
  (*Mathematica definition form → the real definition in Mathematica.*)
```

Here μ is the mean value of the distribution and σ is the standard deviation. About the standard deviation, some usefull descrip - tion can be found in the following link: Click Me (If the link does not work, type in the following address: https://www.dropbox.-com/s/bo2pdshtk4hv9ts/Research_Booklet.docx?dl=0).

1.1.2. Lorentzian Profile

$$l[x\_] := \frac{1}{\pi\gamma}\left[\frac{\gamma^2}{(x - x0)^2 + \gamma^2}\right] \text{(*General form, given in the common mathematical form.*)}$$

```
l[x_] := γ / (π * (x^2 + γ^2)) (*Mathematica definition form → the real definition.*)
```

Here x0 is the location parameter which specifies the peak position of the profile, and it is an analogue to the μ for Gaussian profile. γ is the scale parameter, which specifies the half width at half maximum (HWHM), alternatively 2γ for full width at half maximum (FWHM).

1.1.3. Voigt Profile

Given the Gaussian and Lorentzian profile as above, the Voigt profile can be built up by convoluting the above two profile functions. And without losing generality, the Voigt profile here is only given for the centred profile, which means the centre of the profile peak is at zero.

This is the general mathematical expression for Voigt profile:

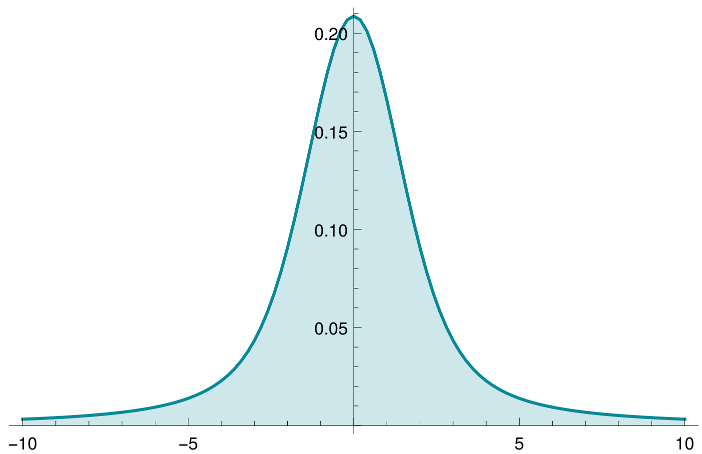
$$v[y\_] := \int_{-\infty}^{\infty} g[y;\ \sigma;\ \mu = 0]\ l[y - x;\ \gamma;\ x0 = 0]\ dx$$

And following is the *Mathematica* expression, in which the *Mathematica* ‘Convolve’ method was used:

```
v[y_] := Convolve[g[x], l[x], x, y]
```

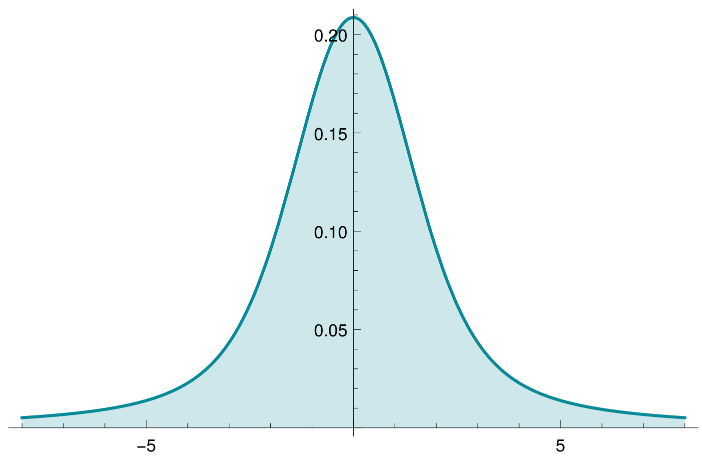
Here is the illustration for Voigt profile, where the parameters value are given as following:

```
σ = 1.00; γ = 1.00;
Voigt`PDF`Arti = Table[{i, v[i]}, {i, -10, 10, 0.2}];
Voigt`PDF`Plot`Arti = ListLinePlot[Voigt`PDF`Arti, Filling → Axis]
```



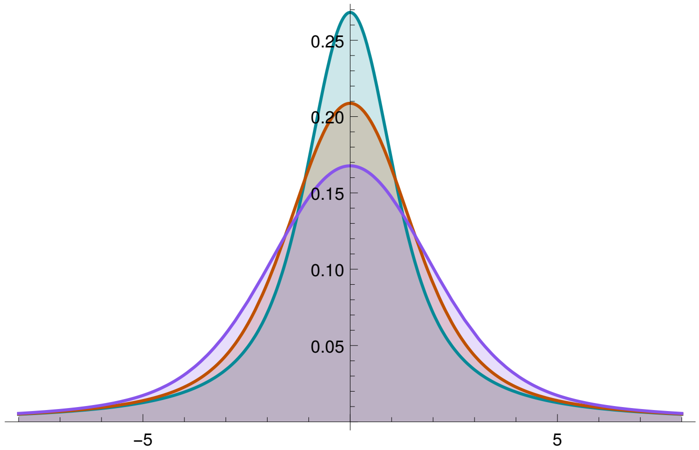
Following is the PDF pattern of Voigt profile which is provided by *Mathematica*. By comparing with the above result, we can see they are exactly (and, naturally) identical to each other.

```
Plot[Evaluate@PDF[VoigtDistribution[1, 1], x],
 {x, -8, 8}, Exclusions → None, Filling → Axis]
```



And here is the illustration for changing the parameters of Voigt profile:

```
Plot[Evaluate@Table[PDF[VoigtDistribution[1, σ], x], {σ, {0.5, 1., 1.5}}],
 {x, -8, 8}, Exclusions → None, Filling → Axis]
```




```
Plot[Evaluate@Table[PDF[VoigtDistribution[gamma, 1], x], {gamma, {0.5, 1., 1.5}}],
 {x, -8, 8}, Exclusions → None, Filling → Axis]
```