1. The file spectrum.dat (downloadable from the Web site) contains the infrared spectrum of an interstellar gas cloud that was obtained recently with the Spitzer Space Observatory. (The first column is the wavelength in micron and the second is the intensity in MJy sr\(^{-1}\), where – for your general edification – 1 Jy (Jansky) is \(10^{-26}\) W cm\(^{-2}\) s\(^{-1}\) Hz\(^{-1}\)).

The spectrum shows spectral line, corresponding the J = 7 – 5 pure rotational transition of molecular hydrogen, superposed on a roughly flat (i.e. wavelength independent) continuum.

Start by plotting the data in your favorite plotting program (always a good first step)

Then write a program that reads in the spectrum and fits a Gaussian line plus continuum:

\[ I_{FIT} = I_C + I_L \exp \left[ - \frac{(\lambda - \lambda_0)^2}{b^2} \right], \]

where the continuum intensity, \(I_C\), the line intensity \(I_L\), the line centroid, \(\lambda_0\), and the line width, \(b\), are 4 parameters to be determined.

In other words, treat this as a 4-D minimization problem, in which you determine what values of \(I_C\), \(I_L\), \(\lambda_0\), and \(b\) minimize the mean square deviation between the data and the fit:

\[ f = \frac{1}{N} \sum_{\text{data points}} (I_{DATA} - I_{FIT})^2 \]

Create a plot showing your best fit superposed on the data.

Try using both the downhill simplex and conjugate gradient method. In each case explore

(1) how quickly does the method converge (if, indeed, it does converge)

(2) how good does you initial guess of each parameter have to be in order for the routine to “find” the solution; in particular, explore what happens if

   (your initial guess of \(\lambda_0\) – optimal value of \(\lambda_0\)) is greater than

   \(\text{few} \times \max (\text{your initial guess of } b, \text{optimal value of } b)\)