

Exploring Fourier Transform Techniques with Mathcad

Document 2: Fourier Transform of an Interferogram

by

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Note: the Automatic Calculation option in the Math menu should NOT be checked.

Objectives:

After completing this exercise, the student should be able to

1. describe why an interferogram contains spectral information,
2. explain why acquiring and transforming a spectrum of greater resolution takes longer, and
3. calculate and understand the origin of the Nyquist wavenumber in a standard FTIR.

Introduction

In an interferometer, a beam of light is split into two beams, each with half the original intensity. These two beams travel paths whose lengths differ by x before recombining to form one beam again. The electromagnetic fields due to light of wavelength λ present in the beam will interfere constructively when $x=n\lambda$, n an integer, and destructively when $x=(n+1/2)\lambda$. Looked at the other way around, light of a given wavelength will contribute to the recombined beam for some values of x but not for others. Therefore, the graph of intensity of the recombined beam vs. the path-length difference x , called an interferogram, contains information about the frequencies present in the beam. In fact, the Fourier transform of the interferogram is a partial frequency spectrum of the light source. If the light passes through an absorber before entering the interferometer, its frequency content is changed, and this information is contained in the interferogram and its Fourier transform. This is the principle of the FTIR.

In this program, we start from a known spectrum, sample it and Fourier-transform it to obtain the interferogram, then transform back and compare the spectrum obtained from the interferogram with the original, with the objective of understanding how sampling and transforming have affected the appearance of the spectrum.

Experimentally, an interferogram is obtained by measuring the light output of an interferometer as a function of path length difference. In FTIR, the beam from an IR-rich light source (e.g. a hot wire) is collimated, then passed through a beam splitter. Half of the light travels from the beam splitter to a fixed mirror and back. The other half travels to a movable mirror and back. The two beams recombine and the intensity is monitored by an IR-sensitive detector as the movable mirror is moved.

The interferogram is sampled by readings taken every 632.8 nm, the wavelength of the reference laser used in the interferometer. The distance moved by the mirror is the only parameter which can be changed in a standard FTIR.

Part 1: Setup

The spectrum is a vector indexed by i ; the interferogram is a vector indexed by j .

$i := 0..m-1$ range variable for interferogram

$\rho = 6.328 \cdot 10^{-5}$ step size for interferometer movement. Units are cm.

$x_i := \rho \cdot i$ position of interferogram for each data point. Units cm

$j := 0.. \frac{m}{2}$ range variable for FT

$w_j := \frac{j + .1}{x_{m-1}}$ wavenumber variable: units cm^{-1}

Part 2: Spectrum

The light source in an infrared spectrometer is a hot wire or bar; its spectral output is simulated here by $\text{source}(w)$, which has the functional form of the Planck distribution for black body radiation. Absorbances caused by a sample in the beam are simulated by bites taken out of the light, using the function $\text{notch}(w,p,hw)$. p is the position of the center of the "absorbance" and hw is its half-width. These won't look like real absorption bands, but they are simple to calculate. The spectrum is now obtained as the product of source and transmittance. Note that this is still a piecewise-continuous function which can be evaluated at any wavenumber.

$$\text{source}(w) := (w)^5 \cdot (e^{.001 \cdot w} - 1)^{-1} \quad \text{Light source spectrum (black body: see question 2.4)}$$

$$\text{notch}(w,p,hw) := (w > p - hw) \cdot (w < p + hw) \quad \text{Notch function = 1 except in the range } p \pm hw$$

$$T(w) := (1 - (\text{notch}(w, 3100, 20) \cdot .8 + \text{notch}(w, 2900, 20) \cdot .5)) \quad \begin{array}{l} \text{Simulated transmittance of sample.} \\ \text{This and the spectrum will be calculated} \\ \text{for each value of } w_j \text{ indexed above.} \end{array}$$

$$\text{spectrum}(w) := \text{source}(w) \cdot T(w)$$

Mathcad notes

1. Exponents are typed as w^5 .
2. The notch function is constructed from logic functions such as $(a > b)$, which equals one if true and 0 if false.

EXERCISES

- 2.1 Where does the number 6.328×10^{-5} cm come from?
- 2.2 The product $\text{source}(w) \cdot T(w)$ is called the "spectrum". What is it the spectrum of?
- 2.3 Compare the functional form of $\text{source}(w)$ to the Planck distribution law. What is λ_{\max} for the function as written?
- 2.4 To what black-body temperature does that wavelength correspond? (hint: find λ_{\max})

$$s0_j := \text{source}(w_j)$$

$s0$ is a digitized (i.e. sampled) spectrum of the light source

$$s_j := \text{spectrum}(w_j)$$

s is a digitized spectrum of the light after passing through an absorbing substance.

The inverse Fourier transform is used to generate the interferograms y and $y0$. These are respectively the interferograms of the light source with and without absorbances.

$$y0 := \text{IFFT}(s0) \quad y := \text{IFFT}(s)$$

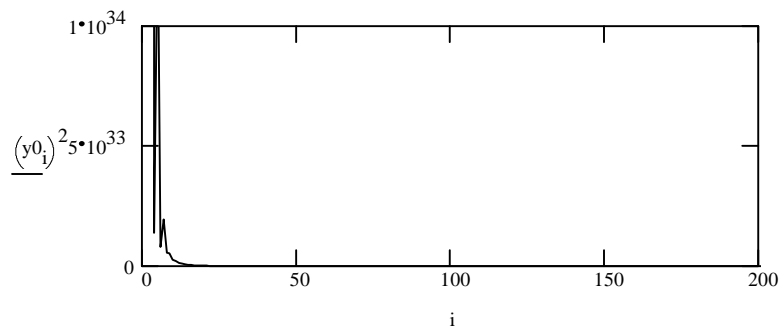
$$Y0 := \text{FFT}(y0) \quad Y := \text{FFT}(y)$$

Part 3: Interferograms

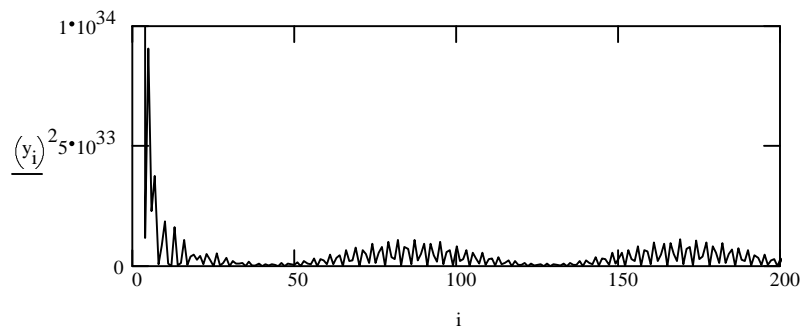
These are graphs of intensity vs interferometer position. The graphs shown here are cut off both vertically and horizontally.

Note that the insertion of a sample in the light beam has produced a noticeable difference in the interferogram. Although it can't be recognized as an absorbance spectrum, absorbance vs. wavelength information is encoded in the interferogram.

Graph 1:
Light source alone.



Graph 2:
With absorbances added.



EXERCISE

2.5 The feature at 0 has a height about 100 times the full scale of the graph. Why is the most intense part of the interferogram at zero?

Part 4: Wavenumber spectrum: FT of interferogram

$$k \equiv 9$$

$$m \equiv 2^k \quad m = \text{number of data points in sample}$$

$$x_{m-1} = 0.032 \quad \text{distance moved by interferometer mirror, in cm}$$

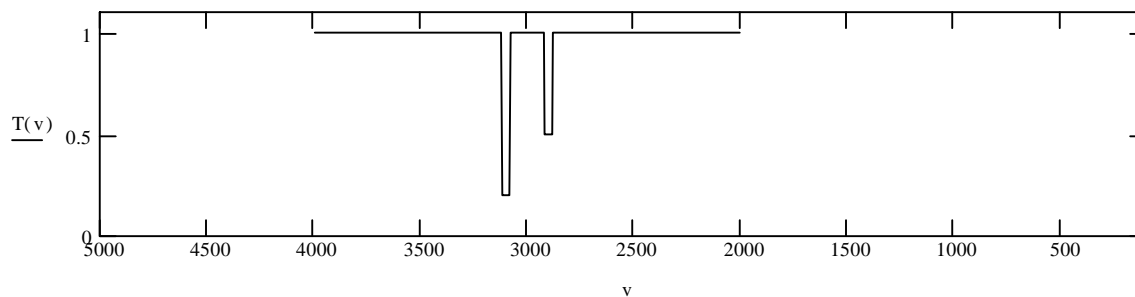
Mathcad notes:

1. Variables defined using $:=$ affect the document only from that point on.
2. Variables defined using \equiv affect the entire document. The regular equals sign $=$ instructs Mathcad to return a value for a variable when the document is calculated.

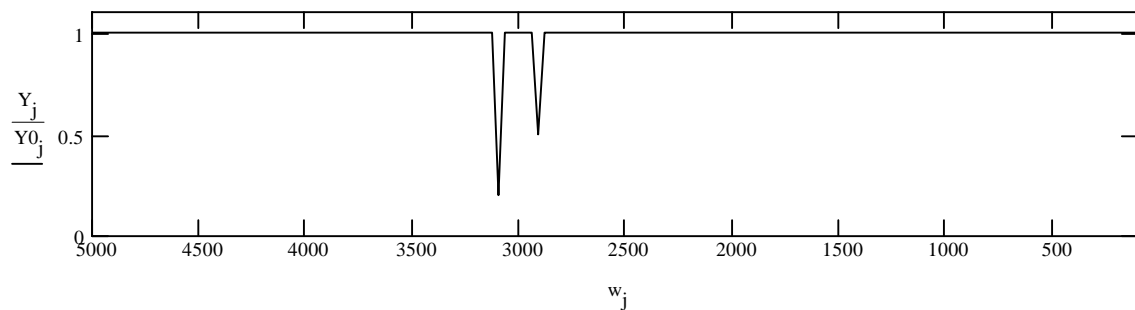
For comparison, the relevant part of the original spectrum is graphed as a function of wavenumber ν .

$$\nu := 2000..4000$$

Graph 3: original transmittance spectrum



Graph 4: wavenumber spectrum: from interferogram



EXERCISES

- 2.6 What is the interval between points on the w axis in the spectrum? (See the equation for w_j in Part 1). This would be quoted as the resolution of the spectrum. What relationship does this resolution have to the distance moved by the mirror?
- 2.7 In order to see the relationship between the distance moved by the mirror and the resolution, move the two peaks closer together by changing their positions in the definition of $T(w)$ above. For example, place the two peaks at 3000 and 2950 (They must remain more than 2 halfwidths apart.) What is the minimum value of k required to distinguish 2 peaks?
- 2.9 By expanding the x -scale of Graph 4 (see tip below), determine the highest frequency which can be observed in the FTIR as set up here. Is this affected by λ or by m ? How?

Mathcad note

To expand the scale of the graph, click on the graph. Locate the axis limits below the left and right ends of the x -axis (5000 and 100) Click on each and press F3 to delete it. Type new limit or leave blank to autoscale. The graph will rescale when F9 is pressed.

- 2.10 Note the default spectral resolution if you have access to an FTIR (if not, use 2 cm^{-1}) and calculate the distance moved by the mirror and the number of data points in the spectrum and transform.
- 2.11 Following usual practice, the spectra in Part 3 have been graphed as sample/reference to remove any spectral features produced by the light source and beam path. Copy Graphs 3 and 4 below; alter the first to show spectrum (that is, s_j vs. w_j) and the second to show Y_j vs. w_j .

Mathcad notes

Click on the graph you wish to copy. The graph should now be boxed. Copy using the Edit menu. Place the cursor in a blank area and paste using the Edit menu or F4.

In order to properly display the resulting graphs, you will have to allow the y -axis to autoscale. Click on the y -axis upper limit 1.1 on the left edge of the graph, press F3 to delete it, then press F9.