Exploring Fourier Transform Techniques with Mathcad
Document 1: Introduction to the Fourier Transform

by

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Notes
1. The Automatic Calculation option under the Math menu should NOT be checked.
2. F9 causes Mathcad to calculate graphs and formulas up to your present position in the document.
3. CTRL R refreshes the window in case some part becomes illegible..

Objectives

After completing the exercises suggested in this document, the student should be able to
1. sketch the FT of a simple waveform;
2. demonstrate or describe why sampling leads to aliasing;
3. determine the Nyquist frequency and predict aliasing;
4. estimate the resolution from the data acquisition time.

Introduction

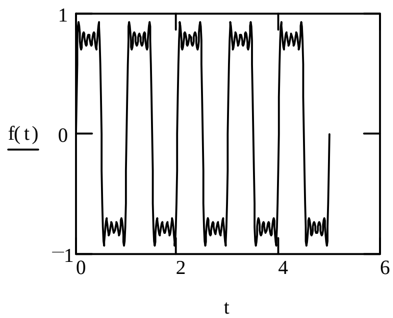
Functions satisfying the Dirichlet conditions (one of which is periodicity) can be written as a sum of a series of sines and cosines, called a Fourier series. For example the sum f(t) below approximates a square wave.

$n := 1, 3 .. 9$ — range for variable n

$\nu := 1$ — fundamental frequency

$f(t) := \sum_{n} n^{-1} \cdot \sin(n \cdot 2 \cdot \pi \cdot \nu \cdot t)$ — definition of function as sum of sines

$t := 0, .01 .. 5$ — range of t for graph



Press F9 to show the graph.

In the reverse of this process, given a waveform, one can determine its frequency makeup by Fourier analysis.

The Fourier Transform

The Fourier transform relates a function to another function of a conjugate variable. The product of the variable and its conjugate is unitless. If t and ω are conjugate variables, then the Fourier transform of f(t) is

$$F(\omega) := (2 \cdot \pi)^{\frac{1}{2}} \cdot \left(\int_{\blacksquare}^{\blacksquare} f(t) \cdot e^{i \cdot \omega \cdot t} \, dt \right)$$

ω is the angular frequency, 2πν. The inverse Fourier transform of F(ω) gives f(t) back:

$$f(t) := (2 \cdot \pi)^{\frac{1}{2}} \cdot \left(\int_{\blacksquare}^{\blacksquare} F(\omega) \cdot e^{-i \cdot \omega \cdot t} \, d\omega \right)$$

For example, if f(t) is a waveform, then F(w) is the contribution of angular frequency w to the waveform. In chemistry, the most common conjugate variable pairs are time/frequency as in this exapmle, and length/wavenumber, which occurs in FTIR.

The Discrete Fourier Transform

Fourier transformations of some functions can be carried out analytically, but in general this is not possible (such as in the case of experimental data). The discrete Fourier transform does not transform the continuous function; it takes a number of evenly-spaced points which sample the function and produces a sample of the transform. Two parameters, the sampling interval and the number of samples, influence the result.

Using time/frequency as an example, suppose a function of time is sampled at intervals τ, that is, at a frequency $1/\tau$, for a total of m samples and a total time of

$$A = m\tau.$$

The highest frequency which will be unambiguously indentified in the transform $F(\omega)$, the Nyquist frequency, is one half of the sampling frequency:

$$\nu_N = 1/(2\tau).$$

Any frequency higher than this will fold back into the interval from 0 to ν_N. The higher frequency is said to be aliased at the lower frequency.

The resolution, the ability to distinguish closely-spaced frequencies, will improve as the sampling time increases. The interval of frequencies from 0 to ν_N covered by $F(\omega)$ is sampled by m/2 points, so the resolution will be no better than

$$\nu_N/(m/2) = 1/A.$$

The fast Fourier transform (FFT) takes advantage of redundancy in the process of calculating a discrete FT to greatly reduce the time required for the calculation. This algorithm and computer hardware implementing it have made FT instruments practical.

Part 1: Sampling and the Nyquist frequency

$t1 := .1, .3 .. 2$

$t := 0, .01 .. 2$

Mathcad notes

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1. An ordinate range must be specified for graphs. In
this case, we have t1:= .1, .3..2  which means that t1
will take on the values 0.1, 0.3 and so on up to 2.
This is typed "t1:.1,.3;2"
2. A second range variable t is also defined. This one
has a spacing small enough to give the appearance of a
continuous graph.
3. Remember to press F9 to calculate the graph.
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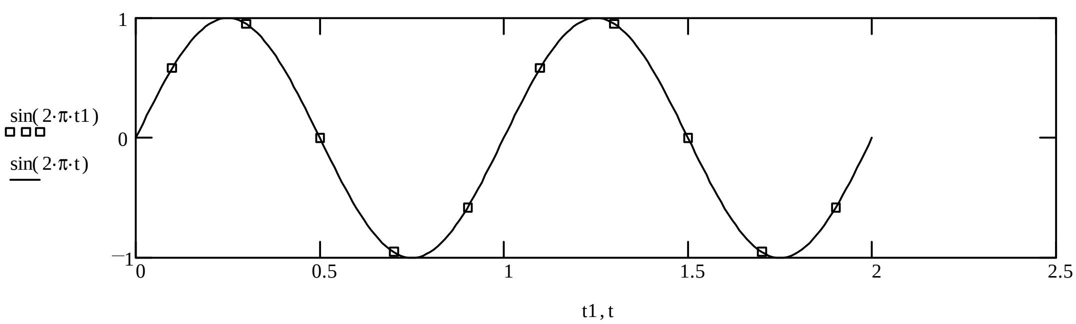
Graph 1

Examine Graph 1. The red line is the graph of a sine function and the blue squares represent samples of this function taken at intervals.



EXERCISES

1.1 Assuming t has units of seconds, what is the frequency of sin(2pt)?
What is its angular frequency?

1.2 Add a third trace to the graph, sin(8pt) vs. t. Given only the blue squares, could the two frequencies be distinguished?

To add a trace to the graph:

Click on sin(2πt), then hit the right arrow until the cursor reaches the end of the expression.
Type comma. This will produce a little black box.
Type "sin(8*CTRL+p*t)"
Press F9

The sampling interval τ determines the highest frequency which can be unambiguously identified. This frequency, equal to $1/2\tau$, is called the Nyquist frequency. Frequencies higher than this will be "aliased" into the range from 0 to $1/2\tau$.

EXERCISE

1.3 Determine the Nyquist frequency for the example above.
(Hint: the variable t1 determines the times of the samples). What is the frequency of sin(8pt)?

Part 2: The Fourier transform

In this part of the program, a waveform (signal vs. time, such as a sound wave or AC voltage) is defined. This waveform is sampled every τ seconds, giving the vector y_i. This vector has m elements which are indexed by the variable i, which runs from 0 to m-1. (The FFT requires an array with 2^n elements). The total sampling time is τm. Each y_i is the intensity of the waveform at the time iτ. The significance of each of these quantities is explored below.

$m := 2^k$ — m = number of data points in sample

$\tau \equiv 10^{-3}$ — τ = sampling interval

$i := 0 .. m-1 \qquad t_i := i \cdot \tau$ — time/s

$y_i := \sin(2 \cdot \pi \cdot \nu 1 \cdot t_i) + \cos(2 \cdot \pi \cdot \nu 2 \cdot t_i)$ — Waveform to be transformed; **y** is a "vector" of data

$j := 0 .. \frac{m}{2} \qquad f_j := \frac{j}{t_{m-1}}$ — frequency/ (s^{-1})

$Y := FFT(y)$ — **Y** is the Fourier transform of **y** (also a vector)

Mathcad notes
If you press F9 at this point, you may notice that the expressions above are briefly highlighted in green as each element of the vector is calculated. That is, a value is calculated for ti and yi for i = 0 to m-1 and to fj for values of j from 0 to m/2. The default value of k is 9, so m = 512.
The Fourier transform of y is also calculated
The frequencies ν1 and ν2 as well as k are `assigned values` in the next section.

Part 3: graphs

The waveform specified above is a sum of a sine and a cosine, with frequencies of ν1 and ν2 respectively. The variable k defines the total number of samples of the waveform which are taken: $m = 2^k$ The total sampling time is t (m-1)

$\nu 1 \equiv 100$ frequencies

$\nu 2 \equiv 110$

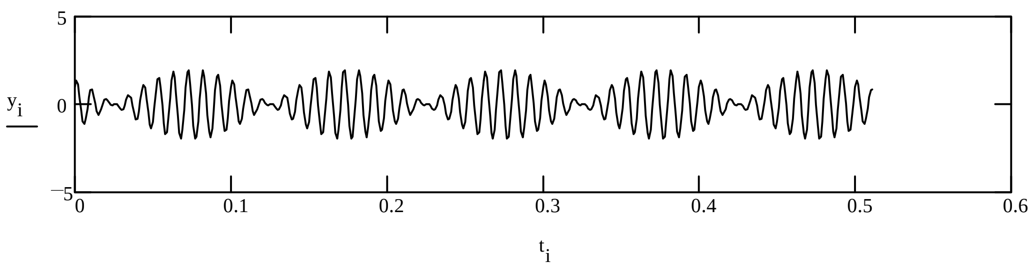
$k \equiv 9$

$m = 512$ number of data points in sample

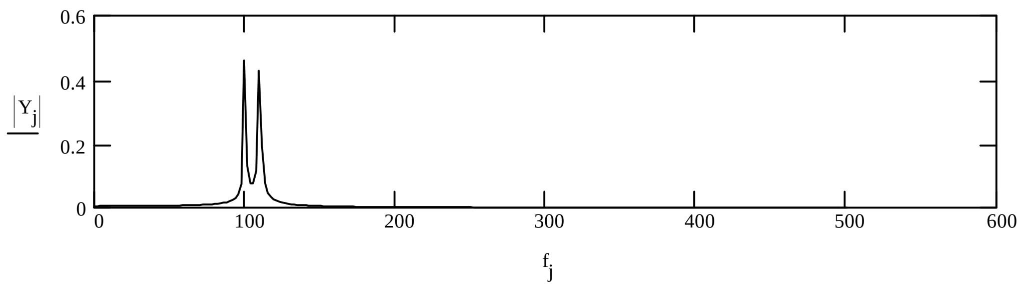
$t_{m-1} = 0.511$ samplng time/s

Graph of waveform y vs. time

Press F9 to see the graphs



Fourier transform of y: frequency spectrum of waveform graphed as amplitude vs. frequency.



Mathcad notes

1. You will be asked to change the values of s, c and k. The easiest way to do this is to click on the current number, press the up arrow until the number is boxed, then press F3. The number will be replaced by a black box. Just type in the new value.
2. F3 is Mathcad's delete key. F4 is the insert key. The last object deleted with F3 can be recovered by pressing F4.
3. If the cursor appears as a vertical line, then backspace or delete can also be used to remove single characters. (Delete acts like backspace.)

Black boxes appearing next to blank graphs indicate that the graph will be autoscaled.

EXERCISES

1.4 Vary s and c to show that Y is the frequency spectrum of y.
1.5 Find the Nyquist frequency for this example.
1.6 Compare c = 400 and c=600. What happens?
1.7 Can you find a rule for the aliasing process? (Hint: the difference between the transformed frequency and the Nyquist frequency are involved.)
1.8 Resolution improves as sampling time increases. Verify this by changing the value of k. Set s to 250 and c to 256. What value of k is required to resolve these two frequencies?
1.9 What is the relationship between the minimum resolvable frequency difference of two components of the signal and the inverse of the total sample time?
1.10 Is there any way to improve resolution without increasing the number of data points? What is the tradeoff?

Part 4: the integral transform

This section is designed to give you an idea of the improvement in speed that the FFT offers. You will set up and calculate an integral transform of the same function to which the FFT was applied above.

$$y(t) := \sin(2\cdot\pi\cdot\nu 1\cdot t) + \cos(2\cdot\pi\cdot\nu 2\cdot t)$$

y(t) is the continuous analogue of the waveform above.

$$Y(f) := \int_0^{\tau\cdot m} y(t)\cdot e^{i\cdot 2\cdot\pi\cdot f\cdot t}\,dt$$

The integral Y(f) is the analytical Fourier transform of y(t).

EXERCISES

1.11 Set c and s back to 100 and 110 respectively. Graph $|Y(f_j)|$ vs f_j .
Press F9 and note the time required for the graph to appear
1.12 Compare the FFT and the integral transform, listing the advantages and limitations of each.

Mathcad notes

Click on a blank spot below. A red + should appear. Define a range for the variable f by typing for example "f:50;150" Click on a blank spot below the range. Create a graph by pressing "@". Type "f" in the little box below the center of the x axis and "|Y(f)" in the little box to the left of the center of the y axis. Press F9 to graph. The green highlighting and the light bulb indicate that a calculation is in progress. The graph will autoscale. Any calculation can be interrupted by pressing ESC.