Understanding the Fourier Transform with Applications to NMR and IR

As you work through the Google Colab notebooks provided, you will be asked a series of questions that you need to complete for this activity. Each question has been reproduced here.

Use this document to complete your assignment by typing your answers directly below each question prompt. Answer all questions completely, explaining your reasoning when appropriate.

Activity 1 Questions

Part 1: Building and plotting waves.

1. Explain in your own words what the plt.grid and plt.legend commands do.
2. What happens when you add the two waves together? Comment on the behavior of the amplitude of the resultant wave. What causes this?

Part 2: Making the connection between sound and notes

2. Which signal is in the time domain? Which one is in the frequency domain?
3. Many people describe the Fourier transform as a "frequency un-mixing machine." How does this example illustrate this idea? Specifically, what is true about the frequencies you set with the sliders and the position of the peaks in the spectrum?
4. In the above function called `update`, you will see a variable `N=120000`. Here, `N` denotes the length of time that we *measure* the audio sine waves. First change the value of `N` to be `N=1200` and re-run the cell containing the `update` function as well as the cell below it that contains `interact(update).`
   a. How does changing this number affect the sound?
   b. How does this change affect the positions and heights of the peaks in the frequency domain?
   c. Repeat these instructions using `N=1200000`. How does this affect the sound and the positions/heights of the peaks in the frequency domain?
   d. What do you predict will happen to the peaks in the frequency domain as we keep making N larger (as N goes to infinity)?
   e. After answering these questions, set `N` back to its original value of `N=120000` in the `update` function.
5. In this example, the peaks look quite different from those we typically encounter in NMR. While revisiting this function, you will also observe that there is a variable called `y_sum` that sums the three waves in this function and is multiplied by a decaying exponential `decaying_exp = np.exp(- 0.0 * time_axis)`. Change the `0.0` to a `0.01` as follows: `decaying_exp = np.exp(- 0.01 * time_axis)`. Then rerun this cell and the cell below.
   a. How does changing this number affect the sound? Compared to the sound you heard in question 4?
   b. How does this affect the shape of the wave called “Sum” in the graph on the left?
      Hint: Replace `ax1.set_xlim(0, 2)` with `ax1.set_xlim(0, 100)`.
   c. How does this change affect the shape of the peaks in the frequency domain?

d. Next, change the `0.01` to a `0.05`. How does this affect the sound?
e. How does this affect the shape of the peaks in the frequency domain?

Part 3: Introducing a quantitative understanding of the FT

6. What are the magnitudes of the Fourier Transform at frequencies of ω = 4 Hz, 6 Hz, 8 Hz, 10 Hz?
7. Justify, qualitatively, why the Fourier Transform evaluated at ω = 10 Hz is different from the others.
8. Without doing any math, what do you expect the Fourier Transform to be when evaluating it at ω = 5 Hz?

Part 4: The Fourier Transform

9. How long does it take to run the Fourier Transform using a resolution of 1/16 Hz? You can find this by looking at the numbers next to the loading bar. For example, if the numbers show `00:02<00:00`, then this means that the calculation took 2 seconds.
10. How much longer does this calculation take using a resolution of 0.001 Hz?
11. What do you notice about the speed of the Fast Fourier Transform (FFT) algorithm? No need to cite a number here–just comment on how fast or slow it is relative to the for-loop based approach.

Part 5: Application to an audio file

12. Using the table provided, label the four prominent peaks in the frequency spectrum of the choir.wav file. What chord is being sung? You may need to use google to look up the name of the chord once you have found the corresponding notes. To narrow down the search, acceptable answers include any combination of {A, B, C, D, E, F, G} and {major, minor}. Hint: the peak frequencies for the four major signals are given in the code used to plot the final figure.

Activity 2 Questions

Part 1: FT-NMR

1. What do you notice about the position of the peaks? How do they relate to the frequencies of the sinusoids you defined above? How does this relate to the results in activity 1?
2. Re-run the above code by changing the amplitude of the input sine waves. How does this affect the resulting spectrum? What happens when the amplitude is doubled? Halved?
3. Recall that the t2* is found in an exponential function: exp(-t/t2*).
   a. What do you expect will happen if you make t2* really large? Test this prediction using the code and note what happens.
   b. What do you expect will happen if you make t2* really small? Test this prediction using the code and note what happens.
4. How does changing the phase (the fourth parameter in `create_wave()`) from zero affect the resulting FT?

Part 2: FT-IR

5. What are the major functional groups in 3-pentanone? Where do you see the transitions corresponding to these functional groups (give the approximate wavenumber of the transition)?
6. Since we are simulating an actual FT-IR experiment, we should think about `tsteps` as the total number of samples we collect, and `dt` as the time between each measurement. Use results from the previous sections to find a sensible value for `dt`. Hint: Find a value `dt` where the wave visually looks smooth.
7. Plot both the `background` and `measured` waves together with limits `(0, 5 * 10e-16)`. What do you observe?
8. Use the space below to plot both the `background_fft` and the `measured_fft` with the corresponding frequency axis you created above with x limits `(0, 1e15)`. What do you observe? Does this look how you would expect?
9. How well does this match the above experimental spectrum of 3-pentanone? Comment on why this predicted spectrum does not resemble the spectrum of 3-pentanone.

Activity 3 Questions

Part 1: Setting Up Our Environment

1. Why do you think the Fourier Transform will not work properly with an enumeration of points?
2. How much energy would a pulse from a 250 MHz NMR instrument contain?
3. On a particular 500 MHz spectrometer, a proton on a molecule produces a frequency of 9.5 kHz and it is known that TMS produces a frequency of 5.9 kHz. What is the equivalent ppm of the unknown proton? What region of a proton NMR does it fall in?
4. What value (in milliseconds) did you get for `dt`?

Part 2: Data Modification and Optimization

5. What is the new duration of the signal? How many data points are in the new signal? Is this a power of 2?
6. What effect did zero-padding have on the FID?
7. Why did we have to calculate a new `time_axis`?
8. Qualitatively, how do the three spectra compare to each other? Specifically discuss differences in peak width, height, resolution. You will want to refer to both the normalized and unnormalized plots to answer this question.
9. In the space below, use the plotting skills you have developed in these activities to zoom into each of the peaks. How many distinct peaks make up each multiplet?
10. Explain how processing the data prior to doing a Fourier transform impacted the resultant spectrum.
11. Of the two individual data processing techniques (zero-padding and windowing), which method yields a higher resolution spectrum?
12. How does the spectrum generated here compare to NMR spectra you are used to seeing from software such as Mnova?
13. In your own words, explain the role of the Fourier Transform in generating an NMR spectrum.

14. Why might collecting data in the time domain be experimentally advantageous compared to collecting data directly in the frequency domain?
15. As mentioned above, you have been working with real experimental NMR data collected on a 500 MHz spectrometer of an unknown compound. Assign the spectrum and determine the identity of the molecule if its chemical formula is C_3H_8O.