Computing Exercise 2: Investigating Simpson's Rule

Saskia Jackson

sj16276

Part a): Simpson's Rule

Simpson's Rule is a simple approximation, used to evaluate integrals that are difficult to calculate using normal integration methods. It is similar to the trapezoidal rule, in that it uses a similar method; splitting up the integral into infinitesimally small segments but is an improvement on the trapezoidal rule as it uses more segments.

Simpson's rule is preferable over the trapezium rule because it converges quicker, meaning that it reaches an accurate answer for the integral in a smaller value of N compared to that of the trapezium rule.

Simpson's rule only works for functions that are smooth over the interval integrated over, therefore a separate function is needed to approximate any periodic functions, whereby the interval is split into smaller intervals. This is called the composite Simpson's rule and mathematically follows the formula:

$$\int_a^b f(x)dx \approx \frac{h}{3}\left[f(x_0) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)\right] \tag{1}$$

where h is the width of each segment and N is the total number of points.

The first part of the exercise is to use Simpson's rule to integrate $\sin(x)$ between 0 and π. This was achieved by defining a function for Simpson's rule by creating two for loops (one for the even functions and one for the odd functions) and adding each term to itself in order to sum the individual functions until the Nth term is added. N is determined by user input, therefore a test must be put in to ensure that the input is a integer and again to ensure it is even. N has to be even so that the limits of the sum are integers.

The function to be integrated was then defined and the final answer printed to the screen.

Number of Iterations	Approximation for sin(x)
4	2.0045597549844207
8	2.0002691699483877
12	2.0000526243411856
16	2.0000165910479355
20	2.000006784441801

Table 1: A table showing how the approximation for $\sin(x)$ varies as the number of iterations increases.

The precise value, calculated as N tends towards infinity, is 2. Therefore it is clear that Simpson's rule is accurate for relatively small values of N.

Part b): Fresnel Diffraction in One Dimension

Simpson's Rule can be applied to many different mathematical problems, wherever an integral is involved. More specifically, in this exercise, it is used to find the electric field of light undergoing Fresnel diffraction.

Fresnel diffraction and the wave theory of light was partially established in the early 19th centary by Augustin-Jean Fresnel and was an advancement on the Huygen principle of light that state that any primary wave front can act as a source for a secondary wavefront. This coupled with interference of wave fronts, can explain the diffraction patterns found in both Fresnel and Fraunhofer.

The integral that needs to be evaluated is a two dimensional integral, integrated over x' and y', the x and y variables on the aperture.

$$E(x, y, z) = \frac{e^{ikz}}{i\lambda z} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} E(x', y') e^{\frac{ik}{2z}[(x-x')^2+(y-y')^2]} dx'dy' \tag{2}$$

where $k = \frac{2\pi}{\lambda}$ and is the wave function, λ is the wavelength of the light, z is the distance between the aperture and the screen and E(x',y') is the electric field of the incident light, which is constant between the aperture limits and zero elsewhere.

This integral can be separated into two one dimensional integrals by setting a variable equal to an integral, allowing the two dimensional integral to become a one dimensional integral.

$$E(x, y, z) = \frac{kE_0}{2\pi z} \int_{y_1'}^{y_2'} X(x, y', z) e^{\frac{ik}{2z}(y-y')^2} dy' \tag{3}$$

where X(x,y',z) is defined below.

$$X(x, y', z) = \int_{x_1'(y')}^{x_2'(y')} e^{\frac{ik}{2z}(x-x')^2} dx' \tag{4}$$

where x and y are the limits of the pattern on the screen and x' and y' are the limits of the aperture.

Part b of the exercise asked for a one dimensional graph of $|X(x, y', z)|^2$ against x. This was achieved by evaluating the integral of $X(x, y', z)$ by defining a function as the exponential in equation 3 with x as the one of the arguments. The graph was then plotted for the modulus of the integration (taken with respect to x') squared against x as it changes in the integral with the x defined in the function equal to the x axis values.

At large distance between the aperture to the screen (anything bigger than around 80mm), Fraunhofer diffraction occurs and thus the graph should resemble a single slit diffraction pattern. This is because from a distance much bigger than the aperture size, the aperture approximates a single slit.

For small z (smaller than roughly 30mm), the diffraction is Fresnel diffraction and therefore the graph has two or more peaks and the minimum points don't reach the x axis.

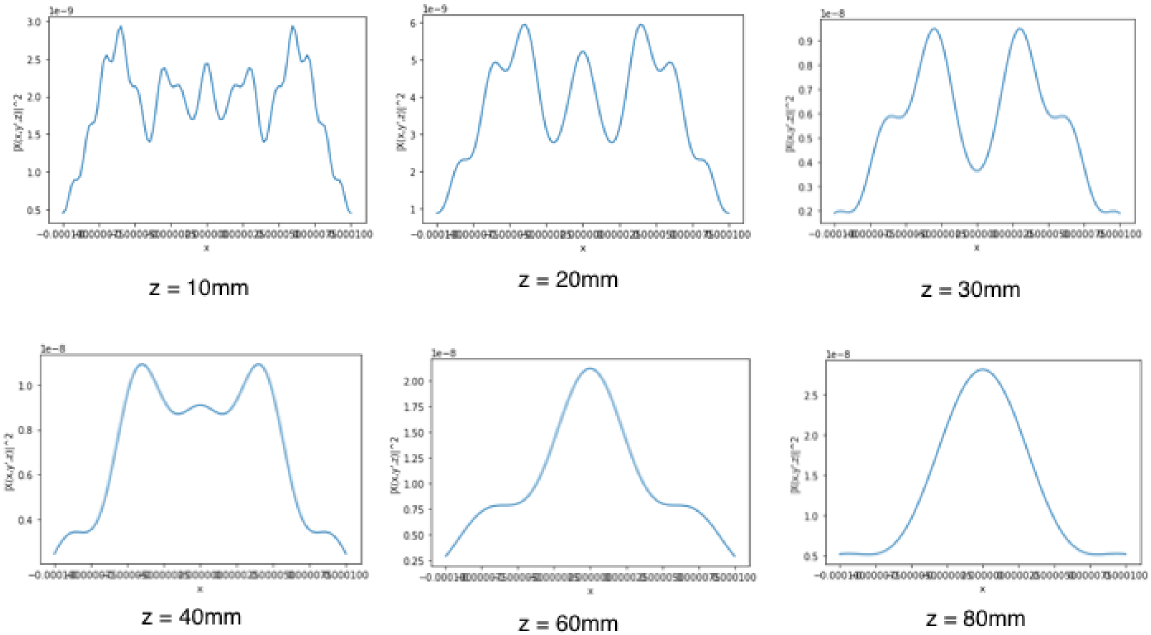

Figure 1: Graphs of $|X(x,y',z)|^2$ against x for $n = 100$ for various values of z from 10mm to 80mm, all taken with N=100 and aperture limits between $\pm 1 \times 10^{-4}$.

If you increase the value for N, the graph becomes more and more accurate as more points are taken in the integral, meaning the increments are much smaller. For example, the following is shows the what the graph looks like at N equal to 10.

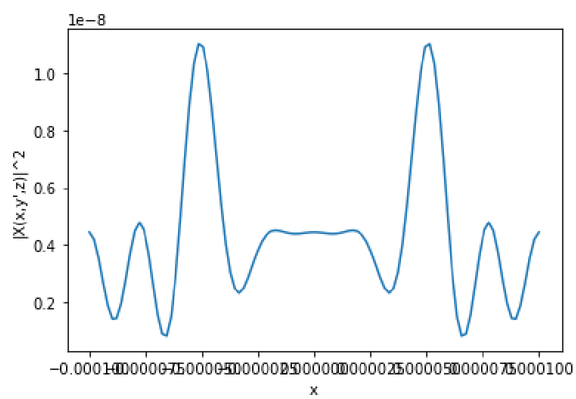

Figure 2: Graphs of $|X(x,y',z)|^2$ against x for $n = 100$ for z=20mm at N=10 and aperture limits between $\pm 1 \times 10^{-4}$.

It is clear from this graph that it neither resembles Fresnel or Fraunhofer due to the small value of N.

Part c): Fresnel Diffraction in Two Dimensions from a Square Aperture

The third part of the exercise asked for a two dimensional intensity plot of Fresnel diffraction for a square aperture. This involved solving the two dimensional integral in equation 3.

The intensity of the light on the screen is determined by the following equation:

$$I(x, y, z) = \epsilon_0 c E(x, y, z) E*(x, y, z) \tag{5}$$

where $E*(x, y, z)$ is the complex conjugate of the electric field.

This was done by defining a function for the x component of the electric field and then running it through a function for the total electric field. Then two for loops are created to set the x and y values to change such that the computer starts at a minimum value of y, then calculates the intensity for each x value, before increasing the y value by one subdivision and repeating the process.

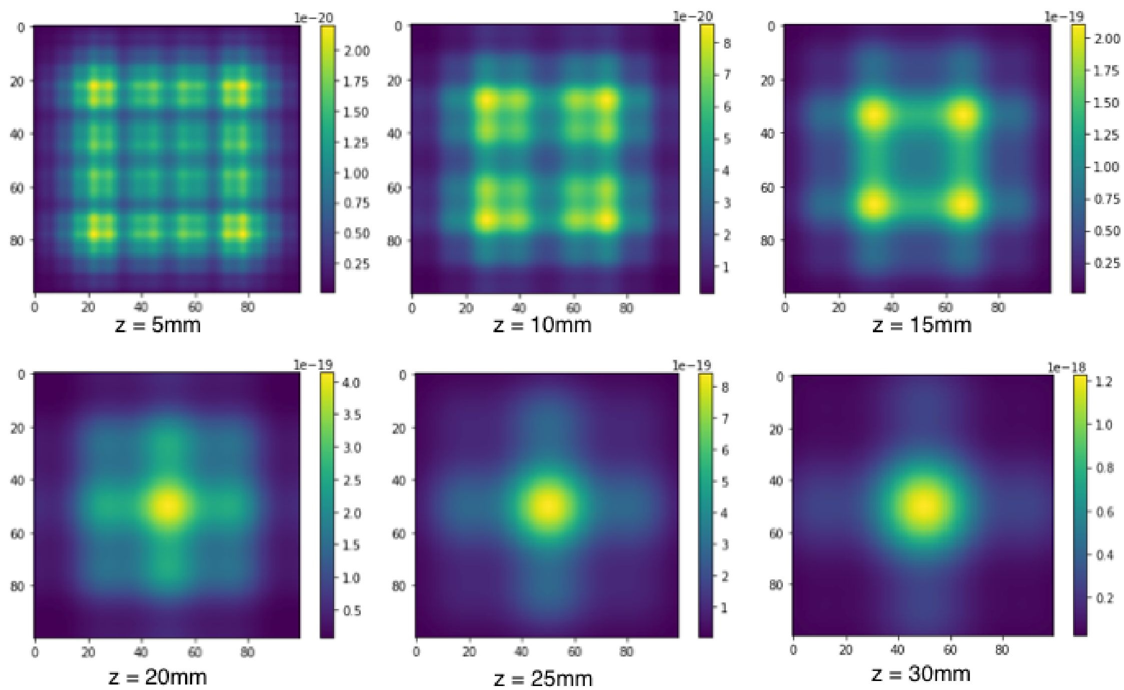

Figure 3: Graphs of diffraction intensity for various values of z from 5mm to 30mm.

At small values of z, most prominently at 5mm, the intensity pattern is more detailed and resembles the size and shape of the aperture more closely compared to the intensity found at much larger distances where the pattern begins to resemble a circular arrangement.

The intensity graphs can be compared to the graphs on the question sheet to ensure they are close to the expected plots.

Part d) Fresnel Diffraction in Two Dimensions from a Circular or Triangular Aperture

Part d of the exercise asks for the code from part c to be altered in order to adapt to triangular or circular apertures.

This can be achieved by setting the aperture limits to be variable dependant on x or y. The limits need to be set to change with the equation of the shape, for example $x = \sqrt{r^2 - y^2}$ for a circular aperture.

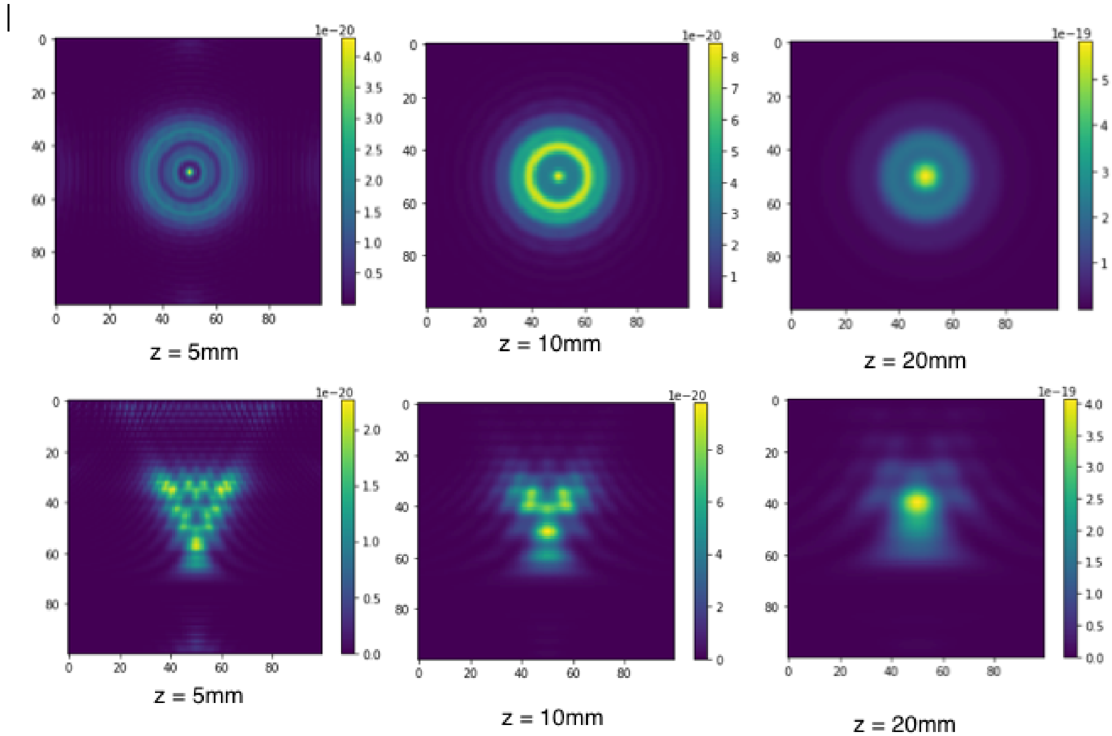

Figure 4: Intensity graphs for triangular and circular aperture for a wavelength of 400nm and an aperture size of $\pm 1 \times 10^{-4}$.

These intensity plots also match the intensity plots found in the questions.

Improvements

One source of error is truncation error which comes from the fact that ideally the limit of the sum would be infinite but in order for realistic approximations to be taken, mostly to reduce the time taken to compute the answers, a finite sum must be taken. This results in a larger error due to some of the part of the sum not being included in the equation. This explains why the graphs in section b are much more accurate for large N.

An alternate method for calculating an integral is the Monte Carlo method. This method is very similar to Simpson's rule but instead of using regular intervals, random points are used instead. It doesn't improve the accuracy of the result by a small amount, but can be very useful for evaluating 4 (or more) dimensional integrals.

Another alternate method is Simpson's 3/8 rule which is very similar to Simpson's rule but multiplies the functions in the sum by three and two, while the whole function is multiplied by $\frac{3h}{8}$ instead of $\frac{h}{3}$. This method is much more accurate than Simpson's rule.

The Romberg method is an alternate method of more accurately approximating the integration by combining the trapezium rule and the midpoint rule, via Richardson extrapolation to get an equation for the integration as:

$$\int_a^b f(x)dx = \frac{h}{2}\left(f(a) + 2\sum_{j=1}^{N-1} f(x_j) + f(b)\right) + \sum_{i=1}^{\infty} K_i h^{2i} \tag{6}$$

This significantly reduces the error found for the integral.