Computational Physics

Exercises for Chapter 5

Exercise 5.1: In the on-line resources you will find a file called `velocities.txt`, which contains two columns of numbers, the first representing time t in seconds and the second the x-velocity in meters per second of a particle, measured once every second from time $t = 0$ to $t = 100$. The first few lines look like this:

```
0         0
1         0.069478
2         0.137694
3         0.204332
4         0.269083
5         0.331656
```

Write a program to do the following:

a) Read in the data and, using the trapezoidal rule, calculate from them the approximate distance traveled by the particle in the x direction as a function of time. See Section 2.4.3 on page 57 if you want a reminder of how to read data from a file.

b) Extend your program to make a graph that shows, on the same plot, both the original velocity curve and the distance traveled as a function of time.

Exercise 5.2:

a) Write a program to calculate an approximate value for the integral $\int_0^2 (x^4 - 2x + 1)\,\mathrm{d}x$ from Example 5.1, but using Simpson's rule with 10 slices instead of the trapezoidal rule. You may wish to base your program on the trapezoidal rule program on page 142.

b) Run the program and compare your result to the known correct value of 4.4. What is the fractional error on your calculation?

c) Modify the program to use a hundred slices instead, then a thousand. Note the improvement in the result. How do the results compare with those from Example 5.1 for the trapezoidal rule with the same numbers of slices?

Exercise 5.3: Consider the integral

$$E(x) = \int_0^x \mathrm{e}^{-t^2}\,\mathrm{d}t.$$

a) Write a program to calculate $E(x)$ for values of x from 0 to 3 in steps of 0.1. Choose for yourself what method you will use for performing the integral and a suitable number of slices.

b) When you are convinced your program is working, extend it further to make a graph of $E(x)$ as a function of x. If you want to remind yourself of how to make a graph, you should consult Section 3.1, starting on page 88.

Note that there is no known way to perform this particular integral analytically, so numerical approaches are the only way forward.

Exercise 5.4: The diffraction limit of a telescope

Our ability to resolve detail in astronomical observations is limited by the diffraction of light in our telescopes. Light from stars can be treated effectively as coming from a point source at infinity. When such light, with wavelength λ, passes through the circular aperture of a telescope (which we'll assume to have unit radius) and is focused by the telescope in the focal plane, it produces not a single dot, but a circular diffraction pattern consisting of central spot surrounded by a series of concentric rings. The intensity of the light in this diffraction pattern is given by

$$I(r) = \left(\frac{J_1(kr)}{kr}\right)^2,$$

where r is the distance in the focal plane from the center of the diffraction pattern, $k = 2\pi/\lambda$, and $J_1(x)$ is a Bessel function. The Bessel functions $J_m(x)$ are given by

$$J_m(x) = \frac{1}{\pi}\int_0^{\pi} \cos(m\theta - x\sin\theta)\,\mathrm{d}\theta,$$

where m is a nonnegative integer and $x \geq 0$.

a) Write a Python function `J(m,x)` that calculates the value of $J_m(x)$ using Simpson's rule with $N = 1000$ points. Use your function in a program to make a plot, on a single graph, of the Bessel functions J_0, J_1, and J_2 as a function of x from $x = 0$ to $x = 20$.

b) Make a second program that makes a density plot of the intensity of the circular diffraction pattern of a point light source with $\lambda = 500\,\text{nm}$, in a square region of the focal plane, using the formula given above. Your picture should cover values of r from zero up to about $1\,\mu\text{m}$.

Hint 1: You may find it useful to know that $\lim_{x\to 0} J_1(x)/x = \frac{1}{2}$. Hint 2: The central spot in the diffraction pattern is so bright that it may be difficult to see the rings around it on the computer screen. If you run into this problem a simple way to deal with it is to use one of the other color schemes for density plots described in Section 3.3. The "`hot`" scheme works well. For a more sophisticated solution to the problem, the `imshow` function has an additional argument `vmax` that allows you to set the value that corresponds to the brightest point in the plot. For instance, if you say "`imshow(x,vmax=0.1)`", then elements in `x` with value 0.1, or any greater value, will produce the brightest (most positive) color on the screen. By lowering the `vmax` value, you can reduce the total range of values between the minimum and maximum brightness, and hence increase the sensitivity of the plot, making subtle details visible. (There is also a `vmin` argument that can be used to set the value that corresponds to the dimmest (most negative) color.) For this exercise a value of `vmax=0.01` appears to work well.

Exercise 5.5: Error on Simpson's rule

Following the same line of argument that led to Eq. (5.28), show that the error on an integral evaluated using Simpson's rule is given, to leading order in h, by Eq. (5.29).

Exercise 5.6: Write a program, or modify an earlier one, to once more calculate the value of the integral $\int_0^2 (x^4 - 2x + 1)\,\mathrm{d}x$ from Example (5.28), using the trapezoidal rule with 20 slices, but this time have the program also print an estimate of the error on the result, calculated using the method of Eq. (5.28). To do this you will need to evaluate the integral twice, once with $N_1 = 10$ slices and then again with $N_2 = 20$ slices. Then Eq. (5.28) gives the error. How does the error calculated in this manner compare with a direct computation of the error as the difference between your value for the integral and the true value of 4.4? Why do the two not agree perfectly?

Exercise 5.7: Consider the integral

$$I = \int_0^1 \sin^2 \sqrt{100x}\,\mathrm{d}x$$

a) Write a program that uses the adaptive trapezoidal rule method of Section 5.3 and Eq. (5.34) to calculate the value of this integral to an approximate accuracy of $\epsilon = 10^{-6}$ (i.e., correct to six digits after the decimal point). Start with one single integration slice and work up from there to two, four, eight, and so forth. Have your program print out the number of slices, its estimate of the integral, and its estimate of the error on the integral, for each value of the number of slices N, until the target accuracy is reached. (Hint: You should find the result is around $I = 0.45$.)

b) Now modify your program to evaluate the same integral using the Romberg integration technique described in this section. Have your program print out a triangular table of values, as on page 161, of all the Romberg estimates of the integral. Calculate the error on your estimates using Eq. (5.49) and again continue the calculation until you reach an accuracy of $\epsilon = 10^{-6}$. You should find that the Romberg method reaches the required accuracy considerably faster than the trapezoidal rule alone.

Exercise 5.8: Write a program that uses the adaptive Simpson's rule method of Section 5.3 and Eqs. (5.35) to (5.39) to calculate the same integral as in Exercise 5.7, again to an approximate accuracy of $\epsilon = 10^{-6}$. Starting this time with two integration slices, work up from there to four, eight, and so forth, printing out the results at each step until the required accuracy is reached. You should find you reach that accuracy for a significantly smaller number of slices than with the trapezoidal rule calculation in part (a) of Exercise 5.7, but a somewhat larger number than with the Romberg integration of part (b).

Exercise 5.9: Heat capacity of a solid

Debye's theory of solids gives the heat capacity of a solid at temperature T to be

$$C_V = 9V\rho k_B \left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{x^4 \mathrm{e}^x}{(\mathrm{e}^x - 1)^2}\,\mathrm{d}x,$$

where V is the volume of the solid, ρ is the number density of atoms, k_B is Boltzmann's constant, and θ_D is the so-called *Debye temperature*, a property of solids that depends on their density and speed of sound.

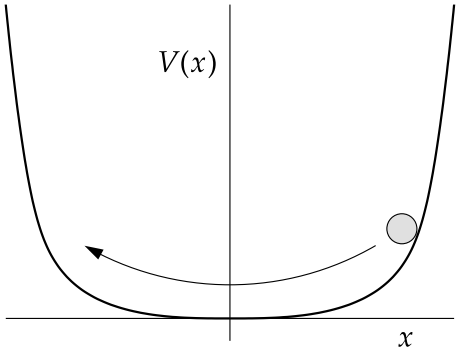
a) Write a Python function `cv(T)` that calculates C_V for a given value of the temperature, for a sample consisting of 1000 cubic centimeters of solid aluminum, which has a number density of $\rho = 6.022 \times 10^{28}\,\mathrm{m}^{-3}$ and a Debye temperature of $\theta_D = 428\,\mathrm{K}$. Use Gaussian quadrature to evaluate the integral, with $N = 50$ sample points.

b) Use your function to make a graph of the heat capacity as a function of temperature from $T = 5\,\mathrm{K}$ to $T = 500\,\mathrm{K}$.

Exercise 5.10: Period of an anharmonic oscillator

The simple harmonic oscillator crops up in many places. Its behavior can be studied readily using analytic methods and it has the important property that its period of oscillation is a constant, independent of its amplitude, making it useful, for instance, for keeping time in watches and clocks. Frequently in physics, however, we also come across anharmonic oscillators, whose period varies with amplitude and whose behavior cannot usually be calculated analytically.

A general classical oscillator can be thought of as a particle in a concave potential well. When disturbed, the particle will rock back and forth in the well:



The harmonic oscillator corresponds to a quadratic potential $V(x) \propto x^2$. Any other form gives an anharmonic oscillator. (Thus there are many different kinds of anharmonic oscillator, depending on the exact form of the potential.)

One way to calculate the motion of an oscillator is to write down the equation for the conservation of energy in the system. If the particle has mass m and position x, then the total energy is equal to the sum of the kinetic and potential energies thus:

$$E = \tfrac{1}{2}m\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 + V(x).$$

Since the energy must be constant over time, this equation is effectively a (nonlinear) differential equation linking x and t.

Let us assume that the potential $V(x)$ is symmetric about $x = 0$ and let us set our anharmonic oscillator going with amplitude a. That is, at $t = 0$ we release it from rest at position

$x = a$ and it swings back towards the origin. Then at $t = 0$ we have $\mathrm{d}x/\mathrm{d}t = 0$ and the equation above reads $E = V(a)$, which gives us the total energy of the particle in terms of the amplitude.

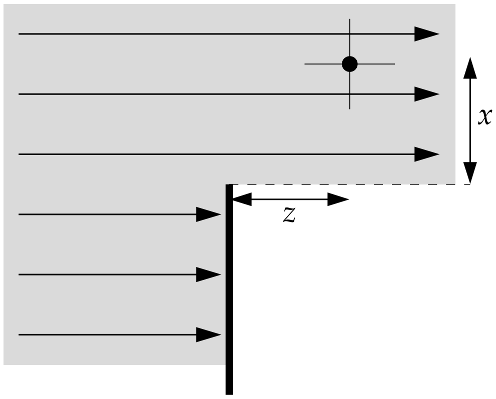
a) When the particle reaches the origin for the first time, it has gone through one quarter of a period of the oscillator. By rearranging the equation above for $\mathrm{d}x/\mathrm{d}t$ and then integrating with respect to t from 0 to $\frac{1}{4}T$, show that the period T is given by

$$T = \sqrt{8m} \int_0^a \frac{\mathrm{d}x}{\sqrt{V(a) - V(x)}}.$$

b) Suppose the potential is $V(x) = x^4$ and the mass of the particle is $m = 1$. Write a Python function that calculates the period of the oscillator for given amplitude a using Gaussian quadrature with $N = 20$ points, then use your function to make a graph of the period for amplitudes ranging from $a = 0$ to $a = 2$.

c) You should find that the oscillator gets faster as the amplitude increases, even though the particle has further to travel for larger amplitude. And you should find that the period diverges as the amplitude goes to zero. How do you explain these results?

Exercise 5.11: Suppose a plane wave, such as light or a sound wave, is blocked by an object with a straight edge, represented by the solid line at the bottom of this figure:



The wave will be diffracted at the edge and the resulting intensity at the position (x, z) marked by the dot is given by near-field diffraction theory to be

$$I = \frac{I_0}{8}\Big(\big[2C(u) + 1\big]^2 + \big[2S(u) + 1\big]^2\Big),$$

where I_0 is the intensity of the wave before diffraction and

$$u = x\sqrt{\frac{2}{\lambda z}}, \qquad C(u) = \int_0^u \cos\tfrac{1}{2}\pi t^2 \,\mathrm{d}t, \qquad S(u) = \int_0^u \sin\tfrac{1}{2}\pi t^2 \,\mathrm{d}t.$$

Write a program to calculate I/I_0 and make a plot of it as a function of x in the range $-5\,\mathrm{m}$ to $5\,\mathrm{m}$ for the case of a sound wave with wavelength $\lambda = 1\,\mathrm{m}$, measured $z = 3\,\mathrm{m}$ past the straight edge. Calculate the integrals using Gaussian quadrature with $N = 50$ points. You should find significant variation in the intensity of the diffracted sound—enough that you could easily hear the effect if sound were diffracted, say, at the edge of a tall building.

Exercise 5.12: The Stefan–Boltzmann constant

The Planck theory of thermal radiation tells us that in the (angular) frequency interval ω to $\omega + \mathrm{d}\omega$, a black body of unit area radiates electromagnetically an amount of thermal energy per second equal to $I(\omega)\,\mathrm{d}\omega$, where

$$I(\omega) = \frac{\hbar}{4\pi^2 c^2} \frac{\omega^3}{(\mathrm{e}^{\hbar\omega/k_B T} - 1)}.$$

Here $\hbar$ is Planck's constant over 2π, c is the speed of light, and k_B is Boltzmann's constant.

a) Show that the total energy per unit area radiated by a black body is

$$W = \frac{k_B^4 T^4}{4\pi^2 c^2 \hbar^3} \int_0^\infty \frac{x^3}{\mathrm{e}^x - 1}\,\mathrm{d}x.$$

b) Write a program to evaluate the integral in this expression. Explain what method you used, and how accurate you think your answer is.

c) Even before Planck gave his theory of thermal radiation around the turn of the 20th century, it was known that the total energy W given off by a black body per unit area per second followed Stefan's law: $W = \sigma T^4$, where σ is the Stefan–Boltzmann constant. Use your value for the integral above to compute a value for the Stefan–Boltzmann constant (in SI units) to three significant figures. Check your result against the known value, which you can find in books or on-line. You should get good agreement.

Exercise 5.13: Quantum uncertainty in the harmonic oscillator

In units where all the constants are 1, the wavefunction of the nth energy level of the one-dimensional quantum harmonic oscillator—i.e., a spinless point particle in a quadratic potential well—is given by

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}}\, \mathrm{e}^{-x^2/2}\, H_n(x),$$

for $n = 0 \ldots \infty$, where $H_n(x)$ is the nth Hermite polynomial. Hermite polynomials satisfy a relation somewhat similar to that for the Fibonacci numbers, although more complex:

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x).$$

The first two Hermite polynomials are $H_0(x) = 1$ and $H_1(x) = 2x$.

a) Write a user-defined function `H(n,x)` that calculates $H_n(x)$ for given x and any integer $n \geq 0$. Use your function to make a plot that shows the harmonic oscillator wavefunctions for $n = 0, 1, 2$, and 3, all on the same graph, in the range $x = -4$ to $x = 4$. Hint: There is a function `factorial` in the `math` package that calculates the factorial of an integer.

b) Make a separate plot of the wavefunction for $n = 30$ from $x = -10$ to $x = 10$. Hint: If your program takes too long to run in this case, then you're doing the calculation wrong—the program should take only a second or so to run.

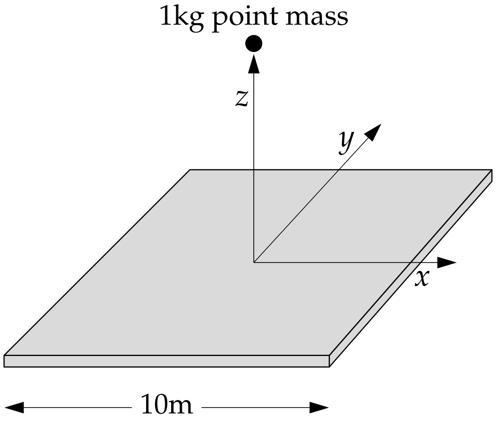
c) The quantum uncertainty of a particle in the nth level of a quantum harmonic oscillator can be quantified by its root-mean-square position $\sqrt{\langle x^2 \rangle}$, where

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi_n(x)|^2 \, \mathrm{d}x.$$

Write a program that evaluates this integral using Gaussian quadrature on 100 points and then calculates the uncertainty (i.e., the root-mean-square position of the particle) for a given value of n. Use your program to calculate the uncertainty for $n = 5$. You should get an answer in the vicinity of $\sqrt{\langle x^2 \rangle} = 2.3$.

Exercise 5.14: Gravitational pull of a uniform sheet

A uniform square sheet of metal is floating motionless in space:



The sheet is 10 m on a side and of negligible thickness, and it has a mass of 10 metric tonnes.

a) Consider the gravitational force due to the plate felt by a point mass of 1 kg a distance z from the center of the square, in the direction perpendicular to the sheet, as shown above. Show that the component of the force along the z-axis is

$$F_z = G\sigma z \iint_{-L/2}^{L/2} \frac{\mathrm{d}x \, \mathrm{d}y}{(x^2 + y^2 + z^2)^{3/2}},$$

where $G = 6.674 \times 10^{-11} \, \mathrm{m}^3 \, \mathrm{kg}^{-1} \, \mathrm{s}^{-2}$ is Newton's gravitational constant and σ is the mass per unit area of the sheet.

b) Write a program to calculate and plot the force as a function of z from $z = 0$ to $z = 10$ m. For the double integral use (double) Gaussian quadrature, as in Eq. (5.82), with 100 sample points along each axis.

c) You should see a smooth curve, except at very small values of z, where the force should drop off suddenly to zero. This drop is not a real effect, but an artifact of the way we have done the calculation. Explain briefly where this artifact comes from and suggest a strategy to remove it, or at least to decrease its size.

This calculation can thought of as a model for the gravitational pull of a galaxy. Most of the mass in a spiral galaxy (such as our own Milky Way) lies in a thin plane or disk passing through the galactic center, and the gravitational pull exerted by that plane on bodies outside the galaxy can be calculated by just the methods we have employed here.

Exercise 5.15: Create a user-defined function `f(x)` that returns the value $1 + \frac{1}{2}\tanh 2x$, then use a central difference to calculate the derivative of the function in the range $-2 \leq x \leq 2$. Calculate an analytic formula for the derivative and make a graph with your numerical result and the analytic answer on the same plot. It may help to plot the exact answer as lines and the numerical one as dots. (Hint: In Python the tanh function is found in the `math` package, and it's called simply `tanh`.)

Exercise 5.16: Even when we can find the value of $f(x)$ for any value of x the forward difference can still be more accurate than the central difference for sufficiently large h. For what values of h will the approximation error on the forward difference of Eq. (5.87) be smaller than on the central difference of Eq. (5.95)?

Exercise 5.17: The gamma function

A commonly occurring function in physics calculations is the gamma function $\Gamma(a)$, which is defined by the integral

$$\Gamma(a) = \int_0^\infty x^{a-1} \mathrm{e}^{-x}\, \mathrm{d}x.$$

There is no closed-form expression for the gamma function, but one can calculate its value for given a by performing the integral above numerically. You have to be careful how you do it, however, if you wish to get an accurate answer.

a) Write a program to make a graph of the value of the integrand $x^{a-1}\mathrm{e}^{-x}$ as a function of x from $x = 0$ to $x = 5$, with three separate curves for $a = 2$, 3, and 4, all on the same axes. You should find that the integrand starts at zero, rises to a maximum, and then decays again for each curve.

b) Show analytically that the maximum falls at $x = a - 1$.

c) Most of the area under the integrand falls near the maximum, so to get an accurate value of the gamma function we need to do a good job of this part of the integral. We can change the integral from 0 to ∞ to one over a finite range from 0 to 1 using the change of variables in Eq. (5.67), but this tends to squash the peak towards the edge of the $[0, 1]$ range and does a poor job of evaluating the integral accurately. We can do a better job by making a different change of variables that puts the peak in the middle of the integration range, around $\frac{1}{2}$. We will use the change of variables given in Eq. (5.69), which we repeat here for convenience:

$$z = \frac{x}{c + x}.$$

For what value of x does this change of variables give $z = \frac{1}{2}$? Hence what is the appropriate choice of the parameter c that puts the peak of the integrand for the gamma function at $z = \frac{1}{2}$?

d) Before we can calculate the gamma function, there is another detail we need to attend to. The integrand $x^{a-1}\mathrm{e}^{-x}$ can be difficult to evaluate because the factor x^{a-1} can become very large and the factor e^{-x} very small, causing numerical overflow or underflow, or both, for some values of x. Write $x^{a-1} = \mathrm{e}^{(a-1)\ln x}$ to derive an alternative expression for the integrand that does not suffer from these problems (or at least not so much). Explain why your new expression is better than the old one.

e) Now, using the change of variables above and the value of c you have chosen, write a user-defined function `gamma(a)` to calculate the gamma function for arbitrary argument a. Use whatever integration method you feel is appropriate. Test your function by using it to calculate and print the value of $\Gamma(\frac{3}{2})$, which is known to be equal to $\frac{1}{2}\sqrt{\pi} \simeq 0.886$.

f) For integer values of a it can be shown that $\Gamma(a)$ is equal to the factorial of $a-1$. Use your Python function to calculate $\Gamma(3)$, $\Gamma(6)$, and $\Gamma(10)$. You should get answers closely equal to $2! = 2$, $5! = 120$, and $9! = 362\,880$.

Exercise 5.18: Rearranging Eq. (5.19) into a slightly more conventional form, we have:

$$\int_a^b f(x)\,\mathrm{d}x = h\biggl[\tfrac{1}{2}f(a) + \tfrac{1}{2}f(b) + \sum_{k=1}^{N-1} f(a+kh)\biggr] + \tfrac{1}{12}h^2\bigl[f'(a) - f'(b)\bigr] + \mathrm{O}(h^4).$$

This result gives a value for the integral on the left which has an error of order h^4—a factor of h^2 better than the error on the trapezoidal rule and as good as Simpson's rule. We can use this formula as a new rule for evaluating integrals, distinct from any of the others we have seen in this chapter. We might call it the "Euler–Maclaurin rule."

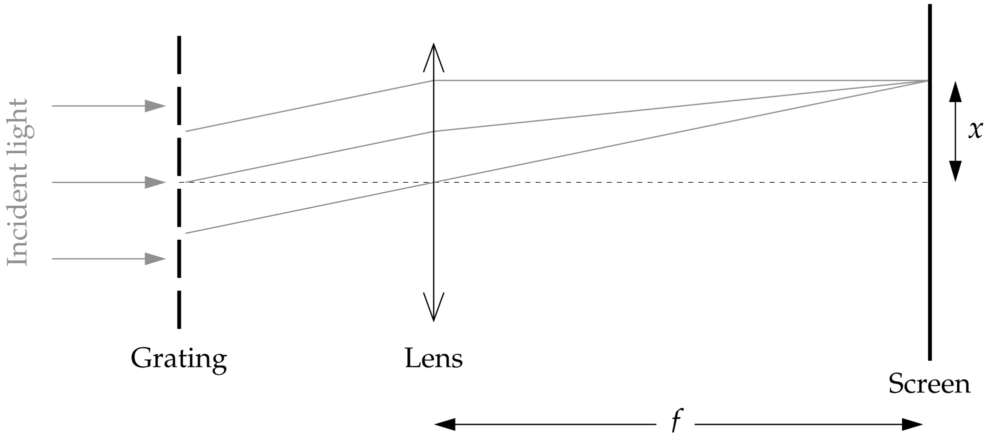
a) Write a program to calculate the value of the integral $\int_0^2 (x^4 - 2x + 1)\,\mathrm{d}x$ using this formula. (This is the same integral that we studied in Example 5.1, whose true value is 4.4.) The order-h term in the formula is just the ordinary trapezoidal rule; the h^2 term involves the derivatives $f'(a)$ and $f'(b)$, which you should evaluate using central differences, centered on a and b respectively. Note that the size of the interval you use for calculating the central differences does not have to equal the value of h used in the trapezoidal rule part of the calculation. An interval of about 10^{-5} gives good values for the central differences.

   Use your program to evaluate the integral with $N = 10$ slices and compare the accuracy of the result with that obtained from the trapezoidal rule alone with the same number of slices.

b) Good though it is, this integration method is not much used in practice. Suggest a reason why not.

Exercise 5.19: Diffraction gratings

Light with wavelength λ is incident on a diffraction grating of total width w, gets diffracted, is focused with a lens of focal length f, and falls on a screen:



Theory tells us that the intensity of the diffraction pattern on the screen, a distance x from the central axis of the system, is given by

$$I(x) = \left| \int_{-w/2}^{w/2} \sqrt{q(u)}\, \mathrm{e}^{\mathrm{i}2\pi x u/\lambda f}\, \mathrm{d}u \right|^2,$$

where $q(u)$ is the intensity transmission function of the diffraction grating at a distance u from the central axis, i.e., the fraction of the incident light that the grating lets through.

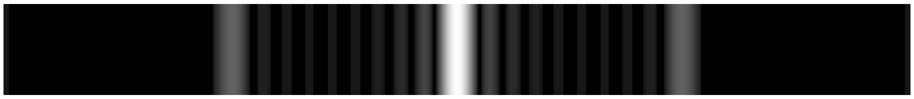
a) Consider a grating with transmission function $q(u) = \sin^2 \alpha u$. What is the separation of the "slits" in this grating, expressed in terms of α?

b) Write a Python function `q(u)` that returns the transmission function $q(u) = \sin^2 \alpha u$ as above at position u for a grating whose slits have separation $20\,\mu$m.

c) Use your function in a program to calculate and graph the intensity of the diffraction pattern produced by such a grating having ten slits in total, if the incident light has wavelength $\lambda = 500\,$nm. Assume the lens has a focal length of 1 meter and the screen is 10 cm wide. You can use whatever method you think appropriate for doing the integral. Once you've made your choice you'll also need to decide the number of sample points you'll use. What criteria play into this decision?

   Notice that the integrand in the equation for $I(x)$ is complex, so you will have to use complex variables in your program. As mentioned in Section 2.2.5, there is a version of the `math` package for use with complex variables called `cmath`. In particular you may find the `exp` function from `cmath` useful because it can calculate the exponentials of complex arguments.

d) Create a visualization of how the diffraction pattern would look on the screen using a density plot (see Section 3.3). Your plot should look something like this:



e) Modify your program further to make pictures of the diffraction patterns produced by gratings with the following profiles:

i) A transmission profile that obeys $q(u) = \sin^2 \alpha u \, \sin^2 \beta u$, with α as before and the same total grating width w, and $\beta = \frac{1}{2}\alpha$.

ii) Two "square" slits, meaning slits with 100% transmission through the slit and 0% transmission everywhere else. Calculate the diffraction pattern for non-identical slits, one 10 μm wide and the other 20 μm wide, with a 60 μm gap between the two.

Exercise 5.20: A more advanced adaptive method for the trapezoidal rule

In Section 5.3 we studied an adaptive version of the trapezoidal rule in which the number of steps is increased—and the width h of the slices correspondingly decreased—until the calculation gives a value for the integral accurate to some desired level. Although this method varies h, it still calculates the integral at any individual stage of the process using slices of equal width throughout the domain of integration. In this exercise we look at a more sophisticated form of the trapezoidal rule that uses different step sizes in different parts of the domain, which can be useful particularly for poorly behaved functions that vary rapidly in certain regions but not others. Remarkably, this method is not much more complicated to program than the ones we've already seen, if one knows the right tricks. Here's how the method works.

Suppose we wish to evaluate the integral $I = \int_a^b f(x) \, dx$ and we want an error of no more than ϵ on our answer. To put that another way, if we divide up the integral into slices of width h then we require an accuracy per slice of

$$h \frac{\epsilon}{b-a} = h\delta,$$

where $\delta = \epsilon/(b-a)$ is the target accuracy per unit interval.

We start by evaluating the integral using the trapezoidal rule with just a single slice of width $h_1 = b - a$. Let us call the estimate of the integral from this calculation I_1. Usually I_1 will not be very accurate, but that doesn't matter. Next we make a second estimate I_2 of the integral, again using the trapezoidal rule but now with two slices of width $h_2 = \frac{1}{2}h_1$ each. Equation (5.28) tells us that the error on this second estimate is $\frac{1}{3}(I_2 - I_1)$ to leading order. If this error is smaller than the required accuracy ϵ then our calculation is complete and we need go no further. I_2 is a good enough estimate of the integral.

Most likely, however, this will not be the case; the accuracy will not be good enough. If so, then we divide the integration interval into two equal parts of size $\frac{1}{2}(b-a)$ each, and we repeat the process above in each part separately, calculating estimates I_1 and I_2 using one and two slices respectively, estimating the error, and checking to see if it is less than the required accuracy, which is now $\frac{1}{2}(b-a)\delta = \frac{1}{2}\epsilon$.

We keep on repeating this process, dividing each slice in half and in half again, as many times as necessary to achieve the desired accuracy in every slice. Different slices may be divided different numbers of times, and hence we may end up with different sized slices in different parts of the integration domain. The method automatically uses whatever size and number of slices is appropriate in each region.

a) Write a program using this method to calculate the integral

$$I = \int_0^{10} \frac{\sin^2 x}{x^2} \, dx,$$

to an accuracy of $\epsilon = 10^{-4}$. Start by writing a function to calculate the integrand $f(x) = (\sin^2 x)/x^2$. Note that the limiting value of the integrand at $x = 0$ is 1. You'll probably have to include this point as a special case in your function using an if statement.

The best way to perform the integration itself is to make use of the technique of recursion, the ability of a Python function to call itself. (If you're not familiar with recursion, you may like to look at Exercise 2.13 on page 83 before doing this exercise.) Write a function `step(x1,x2,f1,f2)` that takes as arguments the beginning and end points x_1, x_2 of a slice and the values $f(x_1), f(x_2)$ of the integrand at those two points, and returns the value of the integral from x_1 to x_2. This function should evaluate the two estimates I_1 and I_2 of the integral from x_1 to x_2, calculated with one and two slices respectively, and the error $\frac{1}{3}(I_2 - I_1)$. If this error meets the target value, which is $(x_2 - x_1)\delta$, then the calculation is complete and the function simply returns the value I_2. If the error fails to meet the target, then the function calls itself, twice, to evaluate the integral separately on the first and second halves of the interval and returns the sum of the two results. (And then *those* functions can call themselves, and so forth, subdividing the integral as many times as necessary to reach the required accuracy.)

Hint: As icing on the cake, when the error target is met and the function returns a value for the integral in the current slice, it can, in fact, return a slightly better value than the estimate I_2. Since you will already have calculated the value of the integrand $f(x)$ at x_1, x_2, and the midpoint $x_m = \frac{1}{2}(x_1 + x_2)$ in order to evaluate I_2, you can use those results to compute the improved Simpson's rule estimate, Eq. (5.7), for this slice. You just return the value $\frac{1}{6}h[f(x_1) + 4f(x_m) + f(x_2)]$ instead of the trapezoidal rule estimate $\frac{1}{4}h[f(x_1) + 2f(x_m) + f(x_2)]$ (where $h = x_2 - x_1$). This involves very little extra work, but gives a value that is more accurate by two orders in h. (Technically, this is an example of the method of "local extrapolation," although it's perhaps not obvious what we're extrapolating in this case. We'll discuss local extrapolation again when we study adaptive methods for the solution of differential equations in Section 8.4.)

b) Why does the function `step(x1,x2,f1,f2)` take not only the positions x_1 and x_2 as arguments, but also the values $f(x_1)$ and $f(x_2)$? Since we know the function $f(x)$, we could just calculate these values from x_1 and x_2. Nonetheless, it is a smart move to include the values of $f(x_1)$ and $f(x_2)$ as arguments to the function. Why?

c) Modify your program to make a plot of the integrand with dots added showing where the ends of each integration slice lie. You should see larger slices in portions of the integrand that follow reasonably straight lines (because the trapezoidal rule gives an accurate value for straight-line integrands) and smaller slices in portions with more curvature.

Exercise 5.21: Electric field of a charge distribution

Suppose we have a distribution of charges and we want to calculate the resulting electric field. One way to do this is to first calculate the electric potential ϕ and then take its gradient. For a point charge q at the origin, the electric potential at a distance r from the origin is $\phi = q/4\pi\epsilon_0 r$ and the electric field is $\mathbf{E} = -\nabla\phi$.

a) You have two charges, of ±1 C, 10 cm apart. Calculate the resulting electric potential on a 1 m × 1 m square plane surrounding the charges and passing through them. Calculate the potential at 1 cm spaced points in a grid and make a visualization on the screen of the potential using a density plot.

b) Now calculate the partial derivatives of the potential with respect to x and y and hence find the electric field in the xy plane. Make a visualization of the field also. This is a little trickier than visualizing the potential, because the electric field has both magnitude and direction. One way to do it might be to make two density plots, one for the magnitude, and one for the direction, the latter using the "`hsv`" color scheme in `pylab`, which is a rainbow scheme that passes through all the colors but starts and ends with the same shade of red, which makes it suitable for representing things like directions or angles that go around the full circle and end up where they started. A more sophisticated visualization might use the arrow object from the `visual` package, drawing a grid of arrows with direction and length chosen to represent the field.

c) Now suppose you have a continuous distribution of charge over an $L \times L$ square. The charge density in Cm^{-2} is

$$\sigma(x,y) = q_0 \sin\frac{2\pi x}{L} \sin\frac{2\pi y}{L}.$$

Calculate and visualize the resulting electric field at 1 cm-spaced points in 1 square meter of the xy plane for the case where $L = 10\,\mathrm{cm}$, the charge distribution is centered in the middle of the visualized area, and $q_0 = 100\,\mathrm{Cm}^{-2}$. You will have to perform a double integral over x and y, then differentiate the potential with respect to position to get the electric field. Choose whatever integration method seems appropriate for the integrals.

Exercise 5.22: Differentiating by integrating

If you are familiar with the calculus of complex variables, you may find the following technique useful and interesting.

Suppose we have a function $f(z)$ whose value we know not only on the real line but also for complex values of its argument. Then we can calculate derivatives of that function at any point z_0 by performing a contour integral, using the Cauchy derivative formula:

$$\left(\frac{\mathrm{d}^m f}{\mathrm{d}z^m}\right)_{z=z_0} = \frac{m!}{2\pi\mathrm{i}} \oint \frac{f(z)}{(z-z_0)^{m+1}}\,\mathrm{d}z,$$

where the integral is performed counterclockwise around any contour in the complex plane that surrounds the point z_0 but contains no poles in $f(z)$. Since numerical integration is significantly easier and more accurate than numerical differentiation, this formula provides us with a method for calculating derivatives—and especially multiple derivatives—accurately by turning them into integrals.

Suppose, for example, that we want to calculate derivatives of $f(z)$ at $z = 0$. Let us apply the Cauchy formula above using the trapezoidal rule to calculate the integral along a circular contour centered on the origin with radius 1. The trapezoidal rule will be slightly different from the version we are used to because the value of the interval h is now a complex number, and moreover is not constant from one slice of the integral to the next—it stays constant in modulus, but its argument changes from one slice to another.

We will divide our contour integral into N slices with sample points z_k distributed uniformly around the circular contour at the positions $z_k = \mathrm{e}^{\mathrm{i}2\pi k/N}$ for $k = 0 \ldots N$. Then the distance between consecutive sample points is

$$h_k = z_{k+1} - z_k = \mathrm{e}^{\mathrm{i}2\pi(k+1)/N} - \mathrm{e}^{\mathrm{i}2\pi k/N},$$

and, introducing the shorthand $g(z) = f(z)/z^{m+1}$ for the integrand, the trapezoidal rule approximation to the integral is

$$\begin{aligned}\oint g(z)\,\mathrm{d}z &\simeq \sum_{k=0}^{N-1} \tfrac{1}{2}\bigl[g(z_{k+1}) + g(z_k)\bigr]\bigl[\mathrm{e}^{\mathrm{i}2\pi(k+1)/N} - \mathrm{e}^{\mathrm{i}2\pi k/N}\bigr] \\ &= \tfrac{1}{2}\Biggl[\sum_{k=0}^{N-1} g(z_{k+1})\,\mathrm{e}^{\mathrm{i}2\pi(k+1)/N} - \sum_{k=0}^{N-1} g(z_k)\,\mathrm{e}^{\mathrm{i}2\pi k/N} \\ &\qquad - \sum_{k=0}^{N-1} g(z_{k+1})\,\mathrm{e}^{\mathrm{i}2\pi k/N} + \sum_{k=0}^{N-1} g(z_k)\,\mathrm{e}^{\mathrm{i}2\pi(k+1)/N}\Biggr].\end{aligned}$$

Noting that $z_N = z_0$, the first two sums inside the brackets cancel each other in their entirety, and the remaining two sums are equal except for trivial phase factors, so the entire expression simplifies to

$$\begin{aligned}\oint g(z)\,\mathrm{d}z &\simeq \tfrac{1}{2}\bigl[\mathrm{e}^{\mathrm{i}2\pi/N} - \mathrm{e}^{-\mathrm{i}2\pi/N}\bigr] \sum_{k=0}^{N-1} g(z_k)\,\mathrm{e}^{\mathrm{i}2\pi k/N} \\ &\simeq \frac{2\pi\mathrm{i}}{N} \sum_{k=0}^{N-1} f(z_k)\,\mathrm{e}^{-\mathrm{i}2\pi km/N},\end{aligned}$$

where we have used the definition of $g(z)$ again. Combining this result with the Cauchy formula, we then have

$$\left(\frac{\mathrm{d}^m f}{\mathrm{d}z^m}\right)_{z=0} \simeq \frac{m!}{N} \sum_{k=0}^{N-1} f(z_k)\,\mathrm{e}^{-\mathrm{i}2\pi km/N}.$$

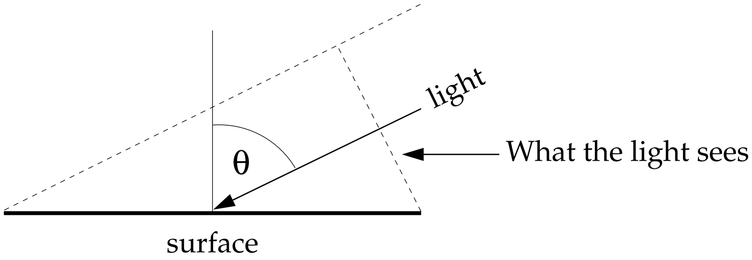
Write a program to calculate the first twenty derivatives of $f(z) = \mathrm{e}^{2z}$ at $z = 0$ using this formula with $N = 10000$. You will need to use the version of the `exp` function from the `cmath` package, which can handle complex arguments. You may also find the function `factorial` from the `math` package useful; it calculates factorials of integer arguments.

The correct value for the mth derivative in this case is easily shown to be 2^m, so it should be straightforward to tell if your program is working—the results should be powers of two, 2, 4, 8, 16, 32, etc. You should find that it is possible to get reasonably accurate results for all twenty derivatives rapidly using this technique. If you use standard difference formulas for the derivatives, on the other hand, you will find that you can calculate only the first three or four derivatives accurately before the numerical errors become so large that the results are useless. In this case, therefore, the Cauchy formula gives the better results.

The sum $\sum_k f(z_k)\,\mathrm{e}^{\mathrm{i}2\pi km/N}$ that appears in the formula above is known as the *discrete Fourier transform* of the complex samples $f(z_k)$. There exists an elegant technique for evaluating the Fourier transform for many values of m simultaneously, known as the *fast Fourier transform*, which could be useful in cases where the direct evaluation of the formula is slow. We will study the fast Fourier transform in detail in Chapter 7.

Exercise 5.23: Image processing and the STM

When light strikes a surface, the amount falling per unit area depends not only on the intensity of the light, but also on the angle of incidence. If the light makes an angle θ to the normal, it only "sees" $\cos\theta$ of area per unit of actual area on the surface:



So the intensity of illumination is $a\cos\theta$, if a is the raw intensity of the light. This simple physical law is a central element of 3D computer graphics. It allows us to calculate how light falls on three-dimensional objects and hence how they will look when illuminated from various angles.

Suppose, for instance, that we are looking down on the Earth from above and we see mountains. We know the height of the mountains $w(x,y)$ as a function of position in the plane, so the equation for the Earth's surface is simply $z = w(x,y)$, or equivalently $w(x,y) - z = 0$, and the normal vector $\mathbf{v}$ to the surface is given by the gradient of $w(x,y) - z$ thus:

$$\mathbf{v} = \nabla[w(x,y) - z] = \begin{pmatrix} \partial/\partial x \\ \partial/\partial y \\ \partial/\partial z \end{pmatrix} [w(x,y) - z] = \begin{pmatrix} \partial w/\partial x \\ \partial w/\partial y \\ -1 \end{pmatrix}.$$

Now suppose we have light coming in represented by a vector $\mathbf{a}$ with magnitude equal to the intensity of the light. Then the dot product of the vectors $\mathbf{a}$ and $\mathbf{v}$ is

$$\mathbf{a}\cdot\mathbf{v} = |\mathbf{a}|\,|\mathbf{v}|\cos\theta,$$

where θ is the angle between the vectors. Thus the intensity of illumination of the surface of the mountains is

$$I = |\mathbf{a}|\cos\theta = \frac{\mathbf{a}\cdot\mathbf{v}}{|\mathbf{v}|} = \frac{a_x(\partial w/\partial x) + a_y(\partial w/\partial y) - a_z}{\sqrt{(\partial w/\partial x)^2 + (\partial w/\partial y)^2 + 1}}.$$

Let's take a simple case where the light is shining horizontally with unit intensity, along a line an angle ϕ counter-clockwise from the east-west axis, so that $\mathbf{a} = (\cos\phi, \sin\phi, 0)$. Then our intensity of illumination simplifies to

$$I = \frac{\cos\phi\,(\partial w/\partial x) + \sin\phi\,(\partial w/\partial y)}{\sqrt{(\partial w/\partial x)^2 + (\partial w/\partial y)^2 + 1}}.$$

If we can calculate the derivatives of the height $w(x, y)$ and we know ϕ we can calculate the intensity at any point.

a) In the on-line resources you'll find a file called `altitude.txt`, which contains the altitude $w(x, y)$ in meters above sea level (or depth below sea level) of the surface of the Earth, measured on a grid of points (x, y). Write a program that reads this file and stores the data in an array. Then calculate the derivatives $\partial w/\partial x$ and $\partial w/\partial y$ at each grid point. Explain what method you used to calculate them and why. (Hint: You'll probably have to use more than one method to get every grid point, because awkward things happen at the edges of the grid.) To calculate the derivatives you'll need to know the value of h, the distance in meters between grid points, which is about 30 000 m in this case. (It's actually not precisely constant because we are representing the spherical Earth on a flat map, but $h = 30\,000$ m will give reasonable results.)

b) Now, using your values for the derivatives, calculate the intensity for each grid point, with $\phi = 45°$, and make a density plot of the resulting values in which the brightness of each dot depends on the corresponding intensity value. If you get it working right, the plot should look like a relief map of the world—you should be able to see the continents and mountain ranges in 3D. (Common problems include a map that is upside-down or sideways, or a relief map that is "inside-out," meaning the high regions look low and *vice versa*. Work with the details of your program until you get a map that looks right to you.)

c) There is another file in the on-line resources called `stm.txt`, which contains a grid of values from scanning tunneling microscope measurements of the (111) surface of silicon. A scanning tunneling microscope (STM) is a device that measures the shape of surfaces at the atomic level by tracking a sharp tip over the surface and measuring quantum tunneling current as a function of position. The end result is a grid of values that represent the height of the surface as a function of position and the data in the file `stm.txt` contain just such a grid of values. Modify the program you just wrote to visualize the STM data and hence create a 3D picture of what the silicon surface looks like. The value of h for the derivatives in this case is around $h = 2.5$ (in arbitrary units).