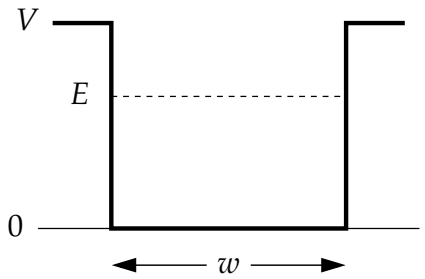
LINEAR AND NON-LINEAR EQUATIONS

FOURIER TRANSFORMS

Homework 4: DUE ON FRIDAY NOVEMBER 4TH AT 11:59 PM

Problem 1: Consider a square potential well of width w, with walls of height V:



Using Schrödinger's equation, it can be shown that the allowed energies E of a single quantum particle of mass m trapped in the well are solutions of

$$\tan\sqrt{w^2mE/2\hbar^2} = \begin{cases} \sqrt{(V-E)/E} & \text{for the even numbered states,} \\ -\sqrt{E/(V-E)} & \text{for the odd numbered states,} \end{cases}$$

where the states are numbered starting from 0, with the ground state being state 0, the first excited state being state 1, and so forth.

a) For an electron (mass 9.1094×10^{-31} kg) in a well with $V = 20$ eV and $w = 1$ nm, write a Python program to plot the three quantities

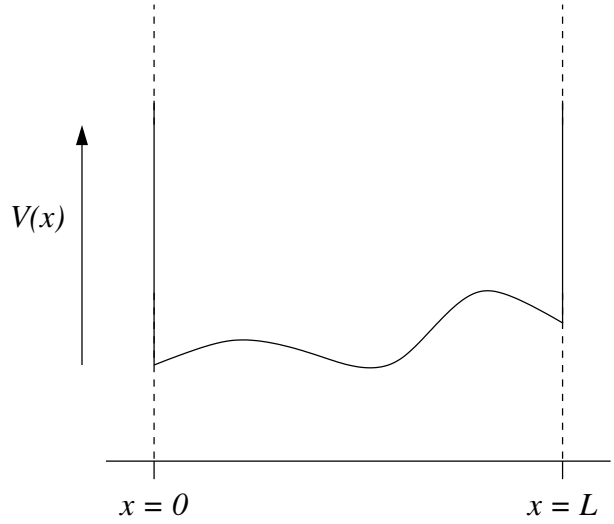
$$y_1 = \tan\sqrt{w^2mE/2\hbar^2}, \qquad y_2 = \sqrt{\frac{V-E}{E}}, \qquad y_3 = -\sqrt{\frac{E}{V-E}},$$

on the same graph, as a function of E from $E = 0$ to $E = 20$ eV. From your plot make approximate estimates of the energies of the first six energy levels of the particle.

b) Write a second program to calculate the values of the first six energy levels in electron volts to an accuracy of 0.001 eV using binary search.

Problem 2: Asymmetric quantum well

Quantum mechanics can be formulated as a matrix problem and solved on a computer using linear algebra methods. Suppose, for example, we have a particle of mass M in a one-dimensional quantum well of width L, but not a square well like the examples you've probably seen before. Suppose instead that the potential $V(x)$ varies somehow inside the well:



We cannot solve such problems analytically in general, but we can solve them on the computer.

In a pure state of energy E, the spatial part of the wavefunction obeys the time-independent Schrödinger equation $\hat{H}\psi(x) = E\psi(x)$, where the Hamiltonian operator $\hat{H}$ is given by

$$\hat{H} = -\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x).$$

For simplicity, let's assume that the walls of the well are infinitely high, so that the wavefunction is zero outside the well, which means it must *go to* zero at $x = 0$ and $x = L$. In that case, the wavefunction can be expressed as a Fourier sine series thus:

$$\psi(x) = \sum_{n=1}^{\infty} \psi_n \sin\frac{\pi n x}{L},$$

where $\psi_1, \psi_2, \ldots$ are the Fourier coefficients. Noting that, for m, n positive integers

$$\int_0^L \sin\frac{\pi m x}{L}\,\sin\frac{\pi n x}{L}\,\mathrm{d}x = \begin{cases} L/2 & \text{if } m = n, \\ 0 & \text{otherwise,} \end{cases}$$

it can be showm that the Schrödinger equation $\hat{H}\psi = E\psi$ implies that

$$\sum_{n=1}^{\infty} \psi_n \int_0^L \sin\frac{\pi m x}{L}\hat{H}\sin\frac{\pi n x}{L}\,\mathrm{d}x = \tfrac{1}{2}LE\psi_m.$$

Hence, defining a matrix $\mathbf{H}$ with elements

$$\begin{aligned} H_{mn} &= \frac{2}{L}\int_0^L \sin\frac{\pi m x}{L}\hat{H}\sin\frac{\pi n x}{L}\,\mathrm{d}x \\ &= \frac{2}{L}\int_0^L \sin\frac{\pi m x}{L}\left[-\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right]\sin\frac{\pi n x}{L}\,\mathrm{d}x, \end{aligned}$$

the Schrödinger's equation can be written in matrix form as $\mathbf{H}\boldsymbol{\psi} = E\boldsymbol{\psi}$, where $\boldsymbol{\psi}$ is the vector $(\psi_1, \psi_2, \ldots)$. Thus $\boldsymbol{\psi}$ is an eigenvector of the *Hamiltonian matrix* $\mathbf{H}$ with eigenvalue E. If we can calculate the eigenvalues of this matrix, then we know the allowed energies of the particle in the well.

a) For the case $V(x) = ax/L$, the integral in H_{mn} can be evaluated analytically to find a general expression for the matrix elements H_{mn} (where the matrix is real and symmetric):

$$H_{mn} = \begin{cases} 0 & \text{if } m \neq n \text{ and both even or both odd,} \\ -\dfrac{8amn}{\pi^2(m^2-n^2)^2} & \text{if } m \neq n \text{ and one is even, one is odd,} \\ \dfrac{a}{2} + \dfrac{\pi^2\hbar^2 m^2}{2ML^2} & \text{if } m = n. \end{cases}$$

Write a Python program to evaluate your expression for H_{mn} for arbitrary m and n when the particle in the well is an electron, the well has width 5 Å, and $a = 10\,\text{eV}$. (The mass and charge of an electron are 9.1094×10^{-31} kg and 1.6022×10^{-19} C respectively.)

b) The matrix **H** is in theory infinitely large, so we cannot calculate all its eigenvalues. But we can get a pretty accurate solution for the first few of them by cutting off the matrix after the first few elements. Modify the program you wrote for part (a) above to create a 10×10 array of the elements of **H** up to $m, n = 10$. Calculate the eigenvalues of this matrix using the appropriate function from `numpy.linalg` and hence print out, in units of electron volts, the first ten energy levels of the quantum well, within this approximation. You should find, for example, that the ground-state energy of the system is around 5.84 eV. (Hint: Bear in mind that matrix indices in Python start at zero, while the indices in standard algebraic expressions, like those above, start at one. You will need to make allowances for this in your program.)

c) Modify your program to use a 100×100 array instead and again calculate the first ten energy eigenvalues. Comparing with the values you calculated in part (c), what do you conclude about the accuracy of the calculation?

d) Now modify your program once more to calculate the wavefunction $\psi(x)$ for the ground state and the first two excited states of the well. Use your results to make a graph with three curves showing the probability density $|\psi(x)|^2$ as a function of x in each of these three states. Pay special attention to the normalization of the wavefunction—it should satisfy the condition $\int_0^L |\psi(x)|^2\,\mathrm{d}x = 1$. Is this true of your wavefunction?

Problem 3: Overrelaxation

Consider the equation $x = 1 - \mathrm{e}^{-cx}$, where c is a known parameter and x is unknown. This equation arises in a variety of situations, including the physics of contact processes, mathematical models of epidemics, and the theory of random graphs.

a) Write a program to solve this equation for x using the relaxation method for the case $c = 2$. Calculate your solution to an accuracy of at least 10^{-6}.

b) Modify your program to calculate the solution for values of c from 0 to 3 in steps of 0.01 and make a plot of x as a function of c. You should see a clear transition from a regime in which $x = 0$ to a regime of nonzero x. This is another example of a phase transition.

In physics this transition is known as the *percolation transition*; in epidemiology it is the *epidemic threshold*.

The ordinary relaxation method involves iterating the equation $x' = f(x)$, starting from an initial guess, until it converges. As we have seen, this is often a fast and easy way to find solutions to nonlinear equations. However, it is possible in some cases to make the method work even faster using the technique of *overrelaxation*. Suppose our initial guess at the solution of a particular equation is, say, $x = 1$, and the final, true solution is $x = 5$. After the first step of the iterative process, we might then see a value of, say, $x = 3$. In the overrelaxation method, we observe this value and note that x is increasing, then we deliberately overshoot the calculated value, in the hope that this will get us closer to the final solution—in this case we might pass over $x = 3$ and go straight to a value of $x = 4$ perhaps, which is closer to the final solution of $x = 5$ and hence should get us to that solution quicker. The overrelaxation method provides a formula for performing this kind of overshooting in a controlled fashion and often, though not always, it does get us to our solution faster. In detail, it works as follows.

We can rewrite the equation $x' = f(x)$ in the form $x' = x + \Delta x$, where

$$\Delta x = x' - x = f(x) - x.$$

The overrelaxation method involves iteration of the modified equation

$$x' = x + (1+\omega)\,\Delta x,$$

(keeping the definition of Δx the same). If the parameter ω is zero, then this is the same as the ordinary relaxation method, but for $\omega > 0$ the method takes the amount Δx by which the value of x would have been changed and changes by a little more. Using $\Delta x = f(x) - x$, we can also write x' as

$$x' = x + (1+\omega)\big[f(x) - x\big] = (1+\omega)f(x) - \omega x,$$

which is the form in which it is usually written.

For the method to work the value of ω must be chosen correctly, although there is some wiggle room—there is an optimal value, but other values close to it will typically also give good results. Unfortunately, there is no general theory that tells us what the optimal value is (usually it is found by trial and error). For the overrelaxation method, it can be shown that the error on x' is given by

$$\epsilon' \simeq \frac{x - x'}{1 - 1/[(1+\omega)f'(x) - \omega]}.$$

c) Consider again the equation $x = 1 - \mathrm{e}^{-cx}$. Take the program you wrote for part (a), which solved the equation for the case $c = 2$, and modify it to print out the number of iterations it takes to converge to a solution accurate to 10^{-6}.

d) Now write a new program (or modify the previous one) to solve the same equation $x = 1 - \mathrm{e}^{-cx}$ for $c = 2$, again to an accuracy of 10^{-6}, but this time using overrelaxation. Have your program print out the answers it finds along with the number of iterations it took to find them. Experiment with different values of ω to see how fast you can get the method to converge. A value of $\omega = 0.5$ is a reasonable starting point. With some trial and error you should be able to get the calculation to converge about twice as fast as the simple relaxation method, i.e., in about half as many iterations.

e) Are there any circumstances under which using a value $\omega < 0$ would help us find a solution faster than we can with the ordinary relaxation method? (Hint: The answer is yes, but why?)

Problem 4: Detecting periodicity

Let's analyze again the data in `sunspots.txt` (from Homework #2), which contains the observed number of sunspots on the Sun for each month since January 1749. The file contains two columns of numbers, the first representing the month and the second being the sunspot number.

a) Write a program that reads the data in the file and makes a graph of sunspots as a function of time. You should see that the number of sunspots has fluctuated on a regular cycle for as long as observations have been recorded. Make an estimate of the length of the cycle in months.

b) Modify your program to calculate the Fourier transform of the sunspot data and then make a graph of the magnitude squared $|c_k|^2$ of the Fourier coefficients as a function of k—also called the *power spectrum* of the sunspot signal. You should see that there is a noticeable peak in the power spectrum at a nonzero value of k. The appearance of this peak tells us that there is one frequency in the Fourier series that has a higher amplitude than the others around it—meaning that there is a large sine-wave term with this frequency, which corresponds to the periodic wave you can see in the original data.

c) Find the approximate value of k to which the peak corresponds. What is the period of the sine wave with this value of k? You should find that the period corresponds roughly to the length of the cycle that you estimated in part (a).

This kind of Fourier analysis is a sensitive method for detecting periodicity in signals. Even in cases where it is not clear to the eye that there is a periodic component to a signal, it may still be possible to find one using a Fourier transform.

Problem 5: Image deconvolution

You've probably seen it on TV, in one of those crime drama shows. They have a blurry photo of a crime scene and they click a few buttons on the computer and magically the photo becomes sharp and clear, so you can make out someone's face, or some lettering on a sign. Surely (like almost everything else on such TV shows) this is just science fiction? Actually, no. It's not. It's real and in this exercise you'll write a program that does it.

When a photo is blurred each point on the photo gets smeared out according to some "smearing distribution," which is technically called a *point spread function*. We can represent this smearing mathematically as follows. For simplicity let's assume we're working with a black and white photograph, so that the picture can be represented by a single function $a(x, y)$ which tells you the brightness at each point (x, y). And let us denote the point spread function by $f(x, y)$. This means that a single bright dot at the origin ends up appearing as $f(x, y)$ instead. If $f(x, y)$ is a broad function then the picture is badly blurred. If it is a narrow peak then the picture is relatively sharp.

In general the brightness $b(x,y)$ of the blurred photo at point (x,y) is given by

$$b(x,y) = \int_0^K \int_0^L a(x',y') f(x-x', y-y')\, \mathrm{d}x'\, \mathrm{d}y',$$

where $K \times L$ is the dimension of the picture. This equation is called the *convolution* of the picture with the point spread function.

Working with two-dimensional functions can get complicated, so to get the idea of how the math works, let's switch temporarily to a one-dimensional equivalent of our problem. Once we work out the details in 1D we'll return to the 2D version. The one-dimensional version of the convolution above would be

$$b(x) = \int_0^L a(x') f(x-x')\, \mathrm{d}x'.$$

The function $b(x)$ can be represented by a Fourier series as in Eq. (7.5):

$$b(x) = \sum_{k=-\infty}^{\infty} \tilde{b}_k \exp\left(\mathrm{i}\frac{2\pi k x}{L}\right),$$

where

$$\tilde{b}_k = \frac{1}{L}\int_0^L b(x) \exp\left(-\mathrm{i}\frac{2\pi k x}{L}\right) \mathrm{d}x$$

are the Fourier coefficients. Substituting for $b(x)$ in this equation gives

$$\begin{aligned}\tilde{b}_k &= \frac{1}{L}\int_0^L \int_0^L a(x') f(x-x') \exp\left(-\mathrm{i}\frac{2\pi k x}{L}\right) \mathrm{d}x'\, \mathrm{d}x \\ &= \frac{1}{L}\int_0^L \int_0^L a(x') f(x-x') \exp\left(-\mathrm{i}\frac{2\pi k (x-x')}{L}\right) \exp\left(-\mathrm{i}\frac{2\pi k x'}{L}\right) \mathrm{d}x'\, \mathrm{d}x.\end{aligned}$$

Now let us change variables to $X = x - x'$, and we get

$$\tilde{b}_k = \frac{1}{L}\int_0^L a(x') \exp\left(-\mathrm{i}\frac{2\pi k x'}{L}\right) \int_{-x'}^{L-x'} f(X) \exp\left(-\mathrm{i}\frac{2\pi k X}{L}\right) \mathrm{d}X\, \mathrm{d}x'.$$

If we make $f(x)$ a periodic function in the standard fashion by repeating it infinitely many times to the left and right of the interval from 0 to L, then the second integral above can be written as

$$\begin{aligned}\int_{-x'}^{L-x'} f(X) \exp\left(-\mathrm{i}\frac{2\pi k X}{L}\right) \mathrm{d}X &= \int_{-x'}^{0} f(X) \exp\left(-\mathrm{i}\frac{2\pi k X}{L}\right) \mathrm{d}X \\ &\qquad + \int_0^{L-x'} f(X) \exp\left(-\mathrm{i}\frac{2\pi k X}{L}\right) \mathrm{d}X \\ &= \exp\left(\mathrm{i}\frac{2\pi k L}{L}\right) \int_{L-x'}^{L} f(X) \exp\left(-\mathrm{i}\frac{2\pi k X}{L}\right) \mathrm{d}X + \int_0^{L-x'} f(X) \exp\left(-\mathrm{i}\frac{2\pi k X}{L}\right) \mathrm{d}X \\ &= \int_0^L f(X) \exp\left(-\mathrm{i}\frac{2\pi k X}{L}\right) \mathrm{d}X,\end{aligned}$$

which is simply L times the Fourier transform $\tilde{f}_k$ of $f(x)$. Substituting this result back into our equation for $\tilde{b}_k$ we then get

$$\tilde{b}_k = \int_0^L a(x') \exp\left(-\mathrm{i}\frac{2\pi k x'}{L}\right) \tilde{f}_k \, \mathrm{d}x' = L\,\tilde{a}_k \tilde{f}_k.$$

In other words, apart from the factor of L, the Fourier transform of the blurred photo is the product of the Fourier transforms of the unblurred photo and the point spread function.

Now it is clear how we deblur our picture. We take the blurred picture and Fourier transform it to get $\tilde{b}_k = L\,\tilde{a}_k \tilde{f}_k$. We also take the point spread function and Fourier transform it to get $\tilde{f}_k$. Then we divide one by the other:

$$\frac{\tilde{b}_k}{L\tilde{f}_k} = \tilde{a}_k$$

which gives us the Fourier transform of the *unblurred* picture. Then, finally, we do an inverse Fourier transform on $\tilde{a}_k$ to get back the unblurred picture. This process of recovering the unblurred picture from the blurred one, of reversing the convolution process, is called *deconvolution*.

Real pictures are two-dimensional, but the mathematics follows through exactly the same. For a picture of dimensions $K \times L$ we find that the two-dimensional Fourier transforms are related by

$$\tilde{b}_{kl} = KL\tilde{a}_{kl}\tilde{f}_{kl}\,,$$

and again we just divide the blurred Fourier transform by the Fourier transform of the point spread function to get the Fourier transform of the unblurred picture.

In the digital realm of computers, pictures are not pure functions $f(x,y)$ but rather grids of samples, and our Fourier transforms are discrete transforms not continuous ones. But the math works out the same again.

The main complication with deblurring in practice is that we don't usually know the point spread function. Typically we have to experiment with different ones until we find something that works. For many cameras it's a reasonable approximation to assume the point spread function is Gaussian:

$$f(x,y) = \exp\left(-\frac{x^2+y^2}{2\sigma^2}\right),$$

where σ is the width of the Gaussian. Even with this assumption, however, we still don't know the value of σ and we may have to experiment to find a value that works well. In the following exercise, for simplicity, we'll assume we know the value of σ.

a) On the web site you will find a file called `blur.txt` that contains a grid of values representing brightness on a black-and-white photo—a badly out-of-focus one that has been deliberately blurred using a Gaussian point spread function of width $\sigma = 25$. Write a program that reads the grid of values into a two-dimensional array of real numbers and then draws the values on the screen of the computer as a density plot. You should see the photo appear. If you get something wrong it might be upside-down. Work with the details of your program until you get it appearing correctly. (Hint: The picture has the sky, which is bright, at the top and the ground, which is dark, at the bottom.)

b) Write another program that creates an array, of the same size as the photo, containing a grid of samples drawn from the Gaussian $f(x, y)$ above with $\sigma = 25$. Make a density plot of these values on the screen too, so that you get a visualization of your point spread function. Remember that the point spread function is periodic (along both axes), which means that the values for negative x and y are repeated at the end of the interval. Since the Gaussian is centered on the origin, this means there should be bright patches in each of the four corners of your picture, something like this:

c) Combine your two programs and add Fourier transforms using the functions `rfft2` and `irfft2` from `numpy.fft`, to make a program that does the following:

i) Reads in the blurred photo
ii) Calculates the point spread function
iii) Fourier transforms both
iv) Divides one by the other
v) Performs an inverse transform to get the unblurred photo
vi) Displays the unblurred photo on the screen

When you are done, you should be able to make out the scene in the photo, although probably it will still not be perfectly sharp.

Hint: One thing you'll need to deal with is what happens when the Fourier transform of the point spread function is zero, or close to zero. In that case if you divide by it you'll get an error (because you can't divide by zero) or just a very large number (because you're dividing by something small). A workable compromise is that if a value in the Fourier transform of the point spread function is smaller than a certain amount ϵ you don't divide by it—just leave that coefficient alone. The value of ϵ is not very critical but a reasonable value seems to be 10^{-3}.

d) Bearing in mind this last point about zeros in the Fourier transform, what is it that limits our ability to deblur a photo? Why can we not perfectly unblur any photo and make it completely sharp?

We have seen this process in action here for a normal snapshot, but it is also used in many physics applications where one takes photos. For instance, it is used in astronomy to enhance

photos taken by telescopes. It was famously used with images from the Hubble Space Telescope after it was realized that the telescope's main mirror had a serious manufacturing flaw and was returning blurry photos—scientists managed to partially correct the blurring using Fourier transform techniques.