AM205: Assignment 5 (due 5 PM, December 2nd)

1. **Rosenbrock function.** A well known benchmark problem for optimization algorithms is minimization of Rosenbrock's function

$$f(x,y) = 100(y-x^2)^2 + (1-x)^2, \tag{1}$$

which has a global minimum of 0 at $(x,y) = (1,1)$. We shall apply three different optimization algorithms for this function; in each case you should terminate the optimization algorithm when the absolute step size falls below 10^{-8}.

   (a) Minimize Rosenbrock's function using steepest descent. You should try the three starting points $[-1,1]^\mathsf{T}$, $[0,1]^\mathsf{T}$, and $[2,1]^\mathsf{T}$, and report the number of iterations required for each starting point. Make a plot for each starting point that shows the contours of Rosenbrock's function, as well as the optimization path that is followed.

   You may use a library function for the line search in steepest descent if you wish. Also, note that steepest descent may require a large number of iterations, so you should terminate the scheme when either the step size tolerance (indicated above) is satisfied, or once 2000 iterations have been performed.

   (b) Repeat part (a), but with Newton's method (without line search) instead of steepest descent.

   (c) Repeat part (a), but with BFGS instead of steepest descent. In your implementation of BFGS, set B_0 to the identity matrix.

2. **Shape determination.** Consider a flexible jump rope of length R that is initially in a vertical xy plane, and hung between the points $(0,0)$ and $(L,0)$. Let the shape of the rope be described parametrically by

$$x(s) = \frac{Ls}{R} + \sum_{k=1}^{20} c_k \sin\frac{\pi k s}{R}, \qquad y(s) = \sum_{k=1}^{20} d_k \sin\frac{\pi k s}{R}, \tag{2}$$

where the coordinate s is the distance along the string when it is unstretched. The jump rope is rotated around the x axis with angular velocity ω. If ρ is the mass per unit unstretched length, its kinetic energy is

$$T = \int_0^R \rho y^2 \omega^2 ds \tag{3}$$

and its elastic potential energy is

$$V = \int_0^R \mu \left(\sqrt{\left(\tfrac{dx}{ds}\right)^2 + \left(\tfrac{dy}{ds}\right)^2} - 1 \right)^2 ds \tag{4}$$

for some stiffness constant μ. Gravitational potential energy is neglected. Using the principle of stationary action, the equilibrium shape of the rope will minimize $V - T$.

Let the vector of parameters be $b = (c_1, c_2, \ldots, c_{20}, d_1, d_2, \ldots, d_{20})$ and let the residual be $r(b) = V - T$, where the integrals in Eqs. 3 and 4 are evaluated at 251 control points using a composite integration rule of your choice.

(a) Determine integral expressions for the components of ∇r.

(b) Using your answer from part (a), write a program to minimize r with respect to b. You may use a library function from Python, Matlab, or other software, although you will need to write the residual function and its gradient. Use the parameters $R = 2$, $\omega = 5$, and $L = \rho = 1$, and use an initial guess of $d_1 = 1$ with the rest of b being zero. On the same axes, plot the shape of the rope for $\mu = 20, 200, 2000$.

(c) For $\mu = 20, 200, 2000$, run your minimization algorithm starting from $d_2 = 0.5$ and all other components of b being zero. Compare your solution with part (b).

(d) **Optional.** Find two friends and a rope. Ask the two friends to each hold one end of the rope, and spin it between them. From a position perpendicular to the spinning axis, take a photo of the rope, trying to catch it at the moment when it is in a vertical plane. By choosing parameters appropriately, superpose one of your calculated curves from on top of the photo, and check the level of agreement. In addition, see if the two friends can recreate the curve from 2(c).

3. **Quantum eigenmodes.** Consider the one-dimensional time-independent Schrödinger equation, which governs the behavior of a quantum particle in a potential well. In non-dimensionalized units where $\frac{\hbar^2}{2m} = 1$, the equation is

$$-\frac{\partial^2 \Psi}{\partial x^2} + v(x)\Psi(x) = E\Psi(x), \tag{5}$$

where $v : \mathbb{R} \to \mathbb{R}$ is a real-valued potential fucntion, $\Psi : \mathbb{R} \to \mathbb{R}$ is the wavefunction, and $E \in \mathbb{R}$ is an eigenvalue which corresponds to the energy of the system. In general, the wave function is complex-valued, but for the time-independent case it is always possible to write it as a real-valued function.

The Schrödinger equation is posed on the infinite domain $(-\infty, \infty)$, and the wavefunction must satisfy $\Psi(x) \to 0$ as $x \to \pm\infty$ so that the norm of Ψ is bounded. In this question, we shall consider the finite interval $[-12, 12]$, which is large enough to impose zero Dirichlet boundary conditions at the boundaries, $\Psi(\pm 12) = 0$, without compromising the accuracy of the results.

As an example of a solution of Eq. 5, in Figure 1 we show the first five eigenvalues and eigenmodes on $x \in [12, 12]$ for the Schrödinger solution in the case that $v(x) = x^2/10$.

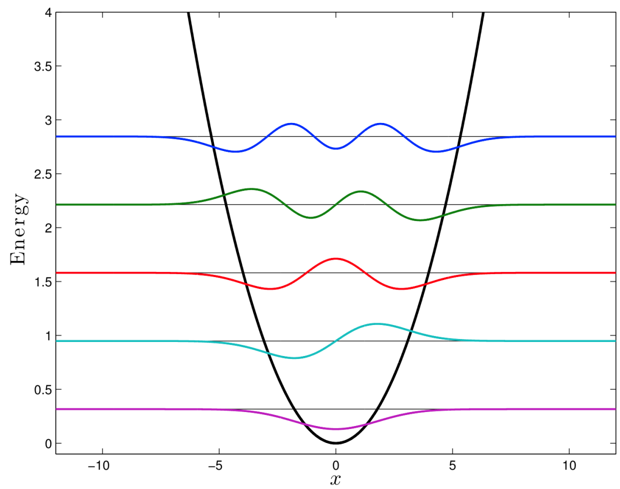
(a) Compute the five lowest eigenvalues and corresponding eigenmodes for the potentials

   i. $v_1(x) = |x|$,

   ii. $v_2(x) = 12\left(\frac{x}{10}\right)^4 - \frac{x^2}{18} + \frac{x}{8} + \frac{13}{10}$,

   iii. $v_3(x) = 8||x| - 1| - 1|$.

You should use a second-order accurate finite-difference apporoximation of Schrödinger equation with $n = 1921$ grids points on the interval $[-12, 12]$, end then employ an eigensolve such as the Python/Matlab `eig`/`eigs` routines. Impose zero boundary conditions at $x = \pm 12$ as described above. Present your results using a figure and a table in the same way as in Figure 1.



E_5	2.846013
E_4	2.213572
E_3	1.581127
E_2	0.948679
E_1	0.316227

Figure 1: The five lowest eigenvalues, and the corresponding eigenmodes, for $v(x) = x^2/10$. To show the eigenmodes in a visually appealing way here we have plotted $y_i(x) = 3\Psi_i(x) + E_i$ for $i = 1, \ldots, 5$.

(b) Quantum mechanics tells us that if a particle has a wavefunction $\Psi(x)$, the the probability of finding it in a region $[a, b]$ is given by

$$\frac{\int_a^b |\Psi(x)|^2 dx}{\int_{-\infty}^{\infty} |\Psi(x)|^2 dx}. \tag{6}$$

For $[a, b] \subset [-12, 12]$ this can be approximated on the finite grid as

$$\frac{\int_a^b |\Psi(x)|^2 dx}{\int_{-12}^{12} |\Psi(x)|^2 dx}. \tag{7}$$

For each of the first five eigenmodes for the potential v_2, use the composite Simpson rule and Eq. 7 to compute the probability that the particle is in the region $x \in [0, 6]$ (*i.e.* specify five different probabilities, one corresponding to each eigenmode). When you use the composite Simpson rule here, you should use all grid points from (a) that are inside the interval of interest as quadrature points.

(c) **Optional.** Modify your program from part (a) to use fourth-order accurate finite differences, using the stencils described on the web, with suitable modifications at the end points.

4. **Pollution scenarios near two factories. (Optional.)** Suppose that there is a school near two industrial factories. In order to develop evacuation procedures for the school, we aim to simulate what happens to pollution that is emitted by the factories. Suppose that plumes of pollution are released simultaneously by the two factories. The concentration of the pollution as a function of position and time, $u(x, t)$, is then governed by the convection–diffusion partial differential equation

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} + [W\cos(\theta), W\sin(\theta)] \cdot \nabla u(\mathbf{x}, t) - 0.05\Delta u(\mathbf{x}, t) = 0, \tag{8}$$

where θ and W are the direction and strength of the wind, respectively. We will model the pollution inside the domain $\Omega = [0,1]^2$, for the time interval $t \in [0, t_f]$ where $t_f = 0.25$. The plumes of pollution at $t = 0$ are described by the initial condition,

$$\begin{aligned} u(\mathbf{x}, 0) = 2 \exp &\left(-150[(x_1 - 0.25)^2 + (x_2 - 0.25)^2]\right) \\ &+ \exp\left(-200[(x_1 - 0.65)^2 + (x_2 - 0.4)^2]\right), \end{aligned} \tag{9}$$

and the pollution is subject to zero Dirichlet boundary conditions,

$$u(\mathbf{x}, t) = 0, \quad \mathbf{x} \in \partial\Omega, \tag{10}$$

for all $t \in [0, t_f]$.

(a) Write a program to solve the convection–diffusion equation using a finite difference method, with a backward Euler discretization in time, and second-order accurate central differences for the spatial derivatives. Throughout this question, use a uniform grid with 81 points in each spatial direction in Ω, and use a time-step $\Delta t = 0.005$.

For the case when $W = 1$ and $\theta = \pi/2$, make contour plots of the pollution concentration profiles at $t = 0$, $t = 0.125$ and $t = 0.25$.

(b) Suppose that the school is at the position $\mathbf{x}_K = (0.5, 0.5)$. Let $k(t; W, \theta) \equiv u(\mathbf{x}_K, t; W, \theta)$ be the pollution level at the school as a function in time, and let $K(W, \theta) \equiv \int_0^{t_f} k(t; W, \theta) dt$ be the total pollution that arrives at the school. From your solution in (a), plot your approximation to $k(t; 1, \pi/2)$ for $t \in [0, t_f]$, and use a composite trapezoid rule to determine $K(1, \pi/2)$.

(c) Determine which wind parameters, W and θ, are maximize $K(W, \theta)$ and are hence the most dangerous for the school.

Suppose that $W \in [0, 3]$ and $\theta \in [0, \pi]$. Use your finite difference approximation along with an optimization routine, using an initial guess of $(W_0, \theta_0) = (1, \pi/2)$, to find the most dangerous wind parameters, W^* and θ^*. What are W^* and θ^*, and what is the corresponding value for $K(W^*, \theta^*)$? Plot $k(t; W^*, \theta^*)$ as a function of time.

(d) Now suppose that the wind speed is fixed to $W = 0.5$, but that the wind direction varies. Suppose that

$$\theta(t) = \sum_{j=0}^{N} \lambda_j T_j \left(\frac{2t}{t_f} - 1\right) \tag{11}$$

where T_j is the jth Chebyshev polynomial, and $\boldsymbol{\lambda} = (\lambda_0, \lambda_1, \ldots, \lambda_N)$ is a vector of parameters. To begin, use $N = 4$. Use a starting guess of $\lambda_0 = \pi/2$ setting all other λ_k equal to zero. Report your value for the total pollution level, $K(\boldsymbol{\lambda}^*)$, and plot $k(t; \boldsymbol{\lambda}^*)$ as a function of time.

(e) Repeat part (d) and try increasing the value of N to examine how the optimal $\theta(t)$ changes.