AM205: Assignment 5 solutions

Problem 1 – Function minimization

The minimization algorithms are tested on the Rosenbrock function,

\[ f(x, y) = 100(y - x^2)^2 + (1 - x)^2. \]  \hspace{1cm} (1)

Part (a) – Steepest descent

The gradient of the function \( f(x, y) \) defined in Eq. 1 is

\[ \nabla f = \begin{pmatrix} -400(y - x^2)x - 2(1 - x) \\ 200(y - x^2) \end{pmatrix}, \]  \hspace{1cm} (2)

and the direction of steepest descent is

\[ s_k = -\nabla f. \]  \hspace{1cm} (3)

We then perform a line search to compute the magnitude of the local descent. It is equivalent of solving a constrained optimization problem. Instead of searching over a two-dimensional domain, we only need to search for the minimum on a line, which is a much simpler computational task. The linear constraint can be written as

\[ A_1 x + A_2 y = b, \]  \hspace{1cm} (4)

and by considering Eq. 3 we know that

\[ A_1 = \frac{\partial f}{\partial y}, \quad A_2 = \frac{\partial f}{\partial x}. \]  \hspace{1cm} (5)

We now solve for \( b \). We have

\[ b = A_1 x_k + A_2 y_k = \frac{\partial f}{\partial y} x_k + \frac{\partial f}{\partial x} y_k. \]  \hspace{1cm} (6)

We then use the Matlab function fmincon to solve the one-dimensional linear search. The Matlab code is as follows.

{[}x_min,f_min,exitflag,output{]}=fmincon(@rosenbrock_function,x_k,{[}{},[],[],[],A,b,[],[],[],[],options)

*Solutions to problems 1 and 3 were written by Kevin Chen (TF, Fall 2014). Solutions to problem 2 was written by Chris H. Rycroft. Edited by Chris H. Rycroft.*
Details can be found in the code problem1aDriver. This process is repeated until the change of consecutive steps is smaller than the tolerance. Figure 1 shows the iterations from three different starting positions. The program is terminated if number of iterations exceeds 2000. For the case of most iteration numbers, we plot the step size versus iterations on a log–log plot to show convergence. The number of iterations we obtain is

\[-1,1]^T \to 2 \text{ iterations},
\[0,1]^T \to \text{more than 2000 iterations},
\[2,1]^T \to 1321 \text{ iterations}.\]
Part (b) – Newton’s method

We repeat part (a) with Newton’s method. To implement Newton’s method, we compute the second derivative (or Hessian matrix) as

$$H = \begin{pmatrix} -400(y - x^2) + 800x^2 + 2 & -400x \\ -400x & 200 \end{pmatrix}. \quad (7)$$

The algorithm is described in the lecture notes, and the key steps inside the loop are

$$H_f(x_k)s_k = -\nabla f(x_k), \quad (8)$$

$$x_{k+1} = x_k + s_k. \quad (9)$$
Figure 3: Plots showing the progress of the BFGS method for finding the minimum of the Rosenbrock function, starting from (top left) $(-1, 1)$, (top right) $(0, 1)$, and (bottom left) $(2, 1)$. In bottom right plot, the step size versus the number of iterations is shown using a log–log scale, for the case of the $(0, 1)$ starting point.

Figure 2 shows the result. In general, this algorithm will converge to local extrema, but not necessarily minima. However, in this problem there is only one local minimum at $(1, 1)$, so we do not need to check for alternative behavior. The number of iterations we obtain is

$[-1, 1]^T \rightarrow 3 \text{ iterations},$  
$[0, 1]^T \rightarrow 6 \text{ iterations},$  
$[2, 1]^T \rightarrow 6 \text{ iterations}.$

**Part (c) – BFGS method**

The BFGS method converges faster than steepest descent but is slower than Newton’s method. Instead of computing the Hessian matrix by hand, we construct an estimate $B$ of
the Hessian, which is continually updated throughout the computation. In this question, we initialize the \( B \) matrix as an identity matrix. The algorithm is detailed in lecture notes. Figure 3 shows the path of convergence for three different initial conditions. Note that the convergence rate is faster than steepest descent but slower than Newton’s method, also the step size is larger at early time. The number of iterations we obtain is

\[
[-1, 1]^T \rightarrow 124 \text{ iterations,} \\
[0, 1]^T \rightarrow 38 \text{ iterations,} \\
[2, 1]^T \rightarrow 45 \text{ iterations.} 
\] (10)

**Problem 2 – a flexible jump rope**

**Part (a) – calculating the Jacobian**

The flexible jump rope can be described parametrically by

\[
x(s) = \frac{Ls}{R} + \sum_{k=1}^{8} c_k \sin \frac{\pi ks}{R}, \quad y(s) = \sum_{k=1}^{8} d_k \sin \frac{\pi ks}{R},
\] (11)

for \( s \in [0, R] \). The first derivatives of these two functions are

\[
\dot{x}(s) = \frac{L}{R} + \frac{\pi}{R} \sum_{k=1}^{8} kc_k \cos \frac{\pi ks}{R}, \quad \dot{y}(s) = \frac{\pi}{R} \sum_{k=1}^{8} kd_k \cos \frac{\pi ks}{R},
\] (12)

where a dot is used to signify a derivative with respect to \( s \). The rope’s shape will minimize the functional

\[
r = V - T = \int_0^R \left( \mu \left( \sqrt{\dot{x}^2 + \dot{y}^2} - 1 \right)^2 - \rho \omega^2 y^2 \right) ds.
\] (13)

The partial derivative of \( r \) with respect to \( c_j \) is

\[
\frac{\partial F}{\partial c_j} = \frac{\pi}{R} \int_0^R \frac{\mu \left( \sqrt{\dot{x}^2 + \dot{y}^2} - 1 \right) 2 \dot{x}j \cos \frac{\pi js}{R}}{\sqrt{\dot{x}^2 + \dot{y}^2}} ds
\] (14)

and the partial derivative of \( r \) with respect to \( d_j \) is

\[
\frac{\partial F}{\partial d_j} = \frac{\pi}{R} \int_0^R \frac{\mu \left( \sqrt{\dot{x}^2 + \dot{y}^2} - 1 \right) 2 \dot{y}j \cos \frac{\pi js}{R}}{\sqrt{\dot{x}^2 + \dot{y}^2}} ds - \frac{2 \rho \omega^2 \pi}{R} \int_0^R yj \sin \frac{\pi js}{R} ds.
\] (15)
Parts (b) and (c)

The code `jump_rope.py` finds the minimum of $r(b)$ using the Levenberg–Marquardt algorithm to set all components of $\nabla r$ to zero. It evaluates the integrals in Eqs. 14 and 15 using the composite trapezoid rule with 251 control points. Figure 4(a) shows a plot of the optimized curves for $\mu = 20, 200, 2000$ starting with $d_1 = 1$ and all other parameters zero. As expected the rope shapes for the lower values of $\mu$ are slightly larger, since the rope can stretch more. Figure 4(b) shows the total amount of stretching as a function of $s$.

Some very small oscillations are visible in Fig. 4, which suggest that using the parameterization in Eq. 11 may not fully resolve the curve. Figure 5 shows the same results when the sums in Eq. 11 are increased from twenty to sixty terms. For this case, the curves appear better resolved.

Figure 6 shows a plot of the optimized curves for $\mu = 20, 200, 2000$ starting with $d_2 = 0.5$ and all other parameters zero. For this case, the code converges to a different minimum that looks like a complete period of a sine wave. Again, the parameterization in Eq. 11 does not appear to fully resolve the curves, and increasing the parameterizations from twenty to sixty terms improves the results, as shown in Fig. 7. As might be expected, the nonlinear functional $r(b)$ defined in Eq. 13 therefore has multiple local minima. While Fig. 4(a) is the typical shape that a jump rope will take, it is also possible to achieve the shape in Fig. 7 through careful spinning.

Problem 3 – quantum eigenmodes

In non-dimensionalized form the Schrödinger equation is

$$ -\frac{\partial^2 \psi(x)}{\partial x^2} + v(x) \psi(x) = E \psi(x). \quad (16) $$

Part (a) – eigenvalues and eigenmodes

We first want to turn the equation into an eigenvalue problem in the form of

$$ A \psi = E \psi, \quad (17) $$

where $A$ is an operator matrix, $\psi$ is a vector and $E$ is a scalar. We discretize the Schrödinger equation on a finite domain $[-12, 12]$ using $n = 1921$ grid points. We use a finite-difference approach, and hence the second-order accurate second-order differentiation matrix is given by

$$ D_2 = \frac{1}{h^2} \begin{pmatrix} -2 & 1 & \cdots & 1 \\ 1 & -2 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \cdots & \cdots & -2 \end{pmatrix}, \quad (18) $$
Figure 4: (a) Shapes of the flexible jump rope for three different elastic constants $\mu$, using the parameterization of Eq. 11; the small circles on the curves are equally spaced in the unstretched coordinate $s$. (b) Stretch factor of the ropes as a function of $s$. \[ \sqrt{\dot{x}^2 + \dot{y}^2} \]
Figure 5: (a) Shapes of the flexible jump rope for three different elastic constants $\mu$, using the parameterization of Eq. 11 but with sixty free parameters instead of twenty; the small circles on the curves are equally spaced in the unstretched coordinate $s$. (b) Stretch factor of the ropes as a function of $s$. 
Figure 6: (a) Shapes of the flexible jump rope for three different elastic constants $\mu$, with the alternative starting guess, using the parameterization of Eq. 11; the small circles on the curves are equally spaced in the unstretched coordinate $s$. (b) Stretch factor of the ropes as a function of $s$. 
Figure 7: (a) Shapes of the flexible jump rope for three different elastic constants $\mu$, with the alternative starting guess, using the parameterization of Eq. 11 but with sixty free parameters instead of twenty; the small circles on the curves are equally spaced in the unstretched coordinate $s$. (b) Stretch factor of the ropes as a function of $s$. 
Figure 8: Five wavefunctions $\Psi_i$ and corresponding energy levels $E_i$ for the potential $v(x) = |x|$.

where $h = 24/(n - 1)$. Since we have Dirichlet boundary conditions and $\Psi(-12) = \Psi(12) = 0$, we do not need to modify the differentiation matrix at the end points. The function $v(x)$ needs to be evaluated at grid points, and therefore needs to be added to the diagonals of the sparse matrix. The operator $A$ can be written as

$$A = -\frac{1}{h^2} \begin{pmatrix} -2 & 1 & \cdots & \cdots & 1 \\ 1 & -2 & \cdots & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & \cdots & \cdots & -2 & 1 \end{pmatrix} + \begin{pmatrix} v(x_1) \\ v(x_1 + h) \\ \vdots \\ v(x_r) \end{pmatrix}. \quad (19)$$

We then use the Matlab function `eigs(A, 5, 'SM')` to find the five smallest eigenvalues and eigenvectors. The eigenvectors are the discretized solution $\Psi_i$ and the eigenvalues are the energy levels $E_i$. For display purposes, we plot $y_i(x) = 3\Psi_i(x) + E_i$. \quad (20)

Figures 8, 9, and 10 show the plots of $\Psi_i$ and tables of the corresponding energy levels.

**Part (b) – probability**

We want to compute the probability of a particle being found in an interval. We know the approximate formula is

$$p = \frac{\int_a^b |\Psi(x)|^2 dx}{\int_{-12}^{12} |\Psi(x)|^2 dx}. \quad (21)$$
Figure 9: Five wavefunctions $\Psi_i$ and corresponding energy levels $E_i$ for the potential $v(x) = 12(x_{10})^4 - \frac{x^2}{18} + \frac{x}{8} + 1.3$.

Figure 10: Five wavefunctions $\Psi_i$ and corresponding energy levels $E_i$ for the potential $v(x) = 8||x| - 1| - 1|$.
We use the composite Simpson’s rule, which has the formula
\[
\int_{a}^{b} f(x) \, dx \approx \frac{h}{3} (f(x_a) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \ldots + 4f(x_{n-1}) + f(x_n)),
\]
where \( h = \frac{2(b - a)}{(n - 1)} \). We integrate over 481 points from \( x = 0 \) to \( x = 6 \). The implementation details are included in function `problem3bDriver`. To four significant figures, the probabilities for the five lowest eigenmodes of potential \( v_2 \) are

- \( E_1 : p(\text{particle} \in [0, 6]) = 0.0003152 \)
- \( E_2 : p(\text{particle} \in [0, 6]) = 0.03036 \)
- \( E_3 : p(\text{particle} \in [0, 6]) = 0.7873 \)
- \( E_4 : p(\text{particle} \in [0, 6]) = 0.3999 \)
- \( E_5 : p(\text{particle} \in [0, 6]) = 0.5325 \)

**Part (c) – fourth-order accurate method**

At an interior point, the fourth-order accurate stencil is
\[
(\Delta x)^2 \frac{\partial^2 \Psi_i}{\partial x^2} \approx -\frac{1}{12} \Psi_{i-2} + \frac{4}{3} \Psi_{i-1} - \frac{5}{2} \Psi_i + \frac{4}{3} \Psi_{i+1} - \frac{1}{12} \Psi_{i+2}.
\]

At the left end point, the fourth-order accurate one-sided stencil,
\[
(\Delta x)^2 \frac{\partial^2 \Psi_1}{\partial x^2} \approx \frac{15}{4} \Psi_1 - \frac{77}{6} \Psi_2 + \frac{107}{6} \Psi_3 - 13 \Psi_4 + \frac{61}{12} \Psi_5 - \frac{5}{6} \Psi_6,
\]

can be used. At the right end point, the same formula can be used but with the grid point ordering reversed to give
\[
(\Delta x)^2 \frac{\partial^2 \Psi_n}{\partial x^2} \approx \frac{15}{4} \Psi_n - \frac{77}{6} \Psi_{n-1} + \frac{107}{6} \Psi_{n-2} - 13 \Psi_{n-3} + \frac{61}{12} \Psi_{n-4} - \frac{5}{6} \Psi_{n-5}.
\]

**Problem 4 – Pollution scenarios near two factories**

The solution to the problem will be added shortly.