

Exercise 1: Electron orbital wave function for the hydrogen atom

The equation for the probability density function of the $n = 3$, $l = 1$, $m = 0$ electron orbital of the hydrogen atom is given as a function of the angle (θ) and radius (r):

$$f(\theta, r) = \left| \frac{\sqrt{2}}{81\sqrt{\pi}} (6r - r^2) e^{-r/3} \cos(\theta) \right|^2$$

where r is in units of the Bohr radius.

- (a) You will begin by making a 3D plot of the function. First, create a mesh grid with θ from 0 to 2π with 0.05π increments, and r from 0 to 20 with 0.5 increments (see `>>help meshgrid`). Assuming you name the resulting matrices **TH** and **R**, then use them to evaluate the above function to find **F** = `f(TH,R)` (make sure your function $f(\theta, r)$ can handle matrix inputs). To plot, first convert the polar-coordinates to cartesian, `[X,Y] = pol2cart(TH,R)`, and then make a 3D plot with `surf(X,Y,F)`. Make sure to comment out this plot before submission to Scorelator. Save **X**, **Y**, and **F** as **A1.dat**, **A2.dat**, and **A3.dat**.
- (b) Looking at the plot in part (a), you should notice that there are four maximums. You will now find the coordinates (θ, r) of these peaks. Using `fminsearch` find the (θ, r) which maximizes $f(\theta, r)$ with each of the following initial guesses: $(0, 1)$, $(0, 10)$, $(\pi, 1)$, and $(\pi, 10)$. Save the resulting (θ, r) values as row vectors in **A4-A7.dat**. Notice how dependent `fminsearch` is on initial conditions.
- (c) Using those same four initial guesses, compute the maxima using Newton's iterative method. We are seeking a zero of:

$$G = \begin{bmatrix} \partial f / \partial \theta \\ \partial f / \partial r \end{bmatrix}.$$

We will also need to make use of the gradient of the gradient of f :

$$D[G] = \begin{bmatrix} \partial^2 f / \partial \theta^2 & \partial^2 f / \partial \theta \partial r \\ \partial^2 f / \partial r \partial \theta & \partial^2 f / \partial r^2 \end{bmatrix}.$$

Newton's iteration for a current guess of $x_k = [\theta_k; r_k]$ is

$$x_{k+1} = x_k - D[G(x_k)]^{-1} [G(x_k)].$$

Compute the matrix inversion $D[G(x_k)]^{-1} [G(x_k)]$ using the backslash notation. Stop iterating when your most recent change $D[G(x_k)]^{-1} [G(x_k)]$ has a two norm that is less than $1e-4$ times the two norm of the current guess x_{k+1} . Save the results as column vectors in **A8-A11.dat**.

Exercise 2: Maximizing Profits

An aircraft manufacturer can produce three different types of aircraft: small, medium, and large. Aircraft costs consist of a materials cost and a labor cost. The small aircraft sells for **\$40 million** more than its materials cost, the medium aircraft sells for **\$ 50 million** more than its materials cost, and the large aircraft sells for **\$75 million** more than its materials cost. Labor cost for each aircraft consists of three parts: fuselage production at **\$32/hour**, wing production at **\$45/hour**, and assembly at **\$30/hour**. Constructing 1 small aircraft requires **.1 million man hours** (mmh) of fuselage production, **.22 mmh** of wing production, and **.15 mmh** of assembly. Constructing 1 medium aircraft requires **.23 mmh** of fuselage production, **.25 mmh** of wing production, and **.17 mmh** of assembly. Constructing one large aircraft requires **.31 mmh** of fuselage production, **.38 mmh** of wing production, and **.27 mmh** of assembly. The following constraints are placed on production:

1. Fuselage production facility can accommodate a maximum of 5 mmh.
2. Wing production facility can accommodate a maximum of 7 mmh.
3. In order to receive a needed tax break, the fuselage production facility must have at least 4 mmh.
4. As they have an overlapping workforce, the combined wing production and assembly labor must not exceed 15 mmh.
5. Due to limited large scale facilities, labor spent on assembly of the large aircraft must not exceed 2 mmh.
6. To fulfill existing contracts, the number of small aircraft produced must be greater than 2.
7. To fulfill existing contracts, the number of medium aircraft produced must be greater than 3.
8. To fulfill existing contracts, the number of large aircraft produced must be greater than 1.

You will be trying to find numbers of small, medium, and large (S , M , and L) aircraft whose production maximizes profit.

- (a) Make a column matrix \mathbf{f} , such that $\mathbf{f}' * [\mathbf{S}; \mathbf{M}; \mathbf{L}]$ is the net profit in millions of dollars (note: this profit should be in millions of dollars, so if the net profit were \$4 million, $\mathbf{f}' * [\mathbf{S}; \mathbf{M}; \mathbf{L}] = 4$). Save as **A12.dat**.
- (b) Make a matrix A and a column vector b such that

$$A \begin{bmatrix} S \\ M \\ L \end{bmatrix} \leq b$$

represents the constraints listed above. Each listed constraint should be represented by the same numbered row of A and b . For example, you should have $A(1,:) = [.1 \ .23 \ .31]$ and $B(1) = 5$. Save A as **A13.dat**, and save b as **A14.dat**.

- (c) Use `linprog` to find $[S; M; L]$. Round each value in the vector to the nearest number and save as **A15.dat**.