

Reading (from Cheney and Kincaid): material from Ch. 14 as on HW # 3

**Assignment:** Do one of the two “Constrained Minimization” choices and one of the two “Optimization” choices. See [www.haverford.edu/math/rmanning/math222/hw.html](http://www.haverford.edu/math/rmanning/math222/hw.html) for notebook with examples of the `If` and `FindMinimum` commands.

**Constrained Minimization:** On Lab # 1, there were several problems that were constrained minimization problems: minimize some function of  $n$  variables  $f(x_1, x_2, \dots, x_n)$  over not all of  $\mathbb{R}^n$ , but some subset of  $\mathbb{R}^n$ . This subset is usually defined by imposing one or more constraint equations  $g(x_1, x_2, \dots, x_n) = 0$ . In Lab # 1, I set these problems up for you so that you did not solve them with minimization algorithms. In this Lab, you will.

### Constrained Minimization Choice 1: Mechanical Equilibrium

Refer to the system of ropes and weights in Lab # 1. Another perspective on this problem is that the angles  $\theta_1$ ,  $\theta_2$ , and  $\theta_3$  will adjust to minimize the combined gravitational potential energy  $E$  of the two masses. Of course, the angles must obey the two constraints

$$\begin{aligned} 3 \cos \theta_1 + 4 \cos \theta_2 + 4 \cos \theta_3 &= 8 \\ 3 \sin \theta_1 - 4 \sin \theta_2 + 4 \sin \theta_3 &= 0 \end{aligned}$$

(In this case, we ignore the tensions). Write an expression for  $E$  as a function of  $\theta_1$  and  $\theta_2$ .

Write a function `energy[theta3_]` which, for a given input value of  $\theta_3$  solves the above system of two constraints for  $\theta_1$  and  $\theta_2$  using Newton’s method, and then plugs those values into  $E$ . (So, the input to `energy` is the angle  $\theta_3$  and the output is the energy  $E$ ; the angles  $\theta_1$  and  $\theta_2$  are computed internally to the function `energy` but are not output by it).

Minimize `energy[theta3]` by a golden section search in Mathematica.

### Constrained Minimization Choice 2: Resource Allocation

Refer back to the ACME Robot Corporation problem in Lab # 1. Recall that we seek to minimize  $C(x, y) = 3x + 5y$  (for convenience, I’ll measure  $C$  in tens of thousands of dollars this time) subject to the constraint that

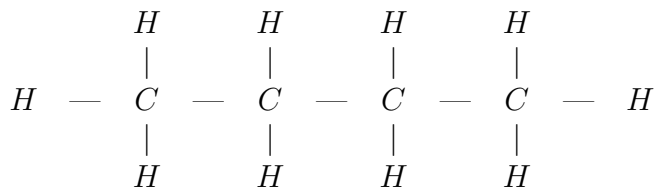
$$S(x, y) = \frac{(15000 - 15000e^{-x/5})(12000 - 12000e^{-y/8})}{10000} = 14000.$$

Write a function `cost[y_]` which, for a given  $y$ , uses Newton’s method to solve the constraint  $S(x, y) = 14000$  for  $x$ , and then plugs this  $(x, y)$  into the cost. (So, the input to `cost` is  $y$  and the output is the cost  $C$ ; the value of  $x$  is computed inside the function `cost` but is not output by it). Note that in this particular problem, you can solve  $S(x, y) = 14000$  for  $x$  in terms of  $y$  by hand or with Mathematica’s `Solve`, but please do it by Newton’s Method (to become more comfortable with Newton’s Method and for uniformity with those doing Choice 1).

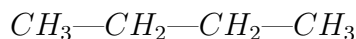
Minimize `cost[y]` by a golden section search in Mathematica.

## Optimization Choice 1: Molecular Mechanics

A simple molecule with more than one energy local minimum is butane,  $C_4H_{10}$ :



We would like to find 3-dimensional configurations that are local minima of the energy, which will certainly not be the ridiculous planar configuration I've drawn here. A molecular modeling package can easily solve this problem by considering all 14 atoms, but that is too strenuous for us to do here. Instead, we will use a simplified model that retains the essence of butane: we will lump each hydrogen in with its nearest carbon (such a "united atom" approach is commonly used in molecular modeling). Thus, our model for butane contains only 4 "atoms":



We will further simplify by assuming that each of the 3 bonds in our simplified model has fixed length 1.52 Angstroms, the equilibrium  $C-C$  bond length (we could easily allow these lengths to vary and include a bond-stretching term if we wanted to).

Choose 3D coordinates so that the first  $CH_2$  lies at  $(0, 0, 0)$ , the second  $CH_2$  lies at  $(1.52, 0, 0)$ , and  $CH_3-CH_2-CH_2$  lies in the  $x-y$  plane. If we let  $\theta$  denote the bond angle  $CH_3-CH_2-CH_2$ , then the first  $CH_3$  lies at  $(1.52 \cos \theta, 1.52 \sin \theta, 0)$ . Two angles are needed to describe the position of the second  $CH_3$ : the bond angle  $CH_2-CH_2-CH_3$ , which we denote by  $\alpha$ , and a "torsion angle"  $\phi$ , which is the angle between the plane containing  $CH_3-CH_2-CH_2$  and the plane containing  $CH_2-CH_2-CH_3$ . In terms of these angles, the position of the second  $CH_3$  is  $(1.52 - 1.52 \cos \alpha, 1.52 \sin \alpha \cos \phi, 1.52 \sin \alpha \sin \phi)$ . Sketch the molecule to make sure you understand these coordinates.

The total energy of a configuration of butane will be the sum of three contributions:

$$E(\theta, \alpha, \phi) = E_{bend} + E_{torsion} + E_{LJ}.$$

The bending energy will be harmonic in each bond angle, centered at the tetrahedral  $109.5^\circ$ :

$$E_{bend} = 47.6 \left( \theta - \frac{109.5\pi}{180} \right)^2 + 47.6 \left( \alpha - \frac{109.5\pi}{180} \right)^2.$$

The interaction of the  $C-H$  and  $C-C$  bonds gives a complicated torsional energy profile:

$$E_{torsion} = 0.0925(1 + \cos \phi) + 0.085(1 + \cos 2\phi) + 0.26(1 + \cos 3\phi).$$

Finally, there is a Lennard-Jones interaction between the two  $CH_3$  units:

$$E_{LJ} = 4(0.027) \left[ \left( \frac{3.63}{r} \right)^{12} - \left( \frac{3.63}{r} \right)^6 \right]$$

where  $r$  is the distance between the two  $CH_3$  units. All coefficients are adaptations of Bowen and Allinger's MM3 force field courtesy of

<http://www.calvin.edu/academic/chemistry/homedocs/compchem/primer/nbpotent.htm>.

**It is crucial that you use radians for all three angles in order for the energies to be correct.**

- (a) Given the positions of the two  $CH_3$  units, compute  $r$  as a function of  $\theta$ ,  $\alpha$ , and  $\phi$ .
- (b) Fix the bond angles  $\alpha$  and  $\theta$  at their equilibrium values  $\frac{109.5\pi}{180}$ . Plot the resulting energy as a function of  $\phi$ . You should find 3 local minima. Locate them numerically using Newton's Method or `FindMinimum`. What do the corresponding physical configurations of butane look like? What are the relative energies of these three configurations?
- (c) Now let the bond angles vary, but assume that  $\alpha = \theta$ . Now the energy is a function of 2 variables:  $\theta$  and  $\phi$ . There should be 3 local minima near the solutions for part (b). Find them with `FindMinimum`. How do they compare (in terms of energy and in terms of configuration) to the solutions from part (b)? Make a contour plot of the energy in the range  $\frac{103\pi}{180} \leq \theta \leq \frac{115\pi}{180}$ ,  $0 \leq \phi \leq 2\pi$ . Use the energies of your local minima to choose contour levels so the three local minima can be deduced from your contour plot.

## Optimization Choice 2: Optimal Portfolio

You have \$ 1 million to invest in any of four investments. Historically, these investments have had average yearly returns of 6, 11, 13, and 18 %, with standard deviations of 2, 15, 15, and 25 % respectively. If we assume that the performance of the different investments are independent, then standard probability theory tells us that if we invest  $w_1, w_2, w_3, w_4$  (in millions of dollars) in these four choices, we expect our total portfolio to have an average yearly return of  $\mu = 0.06w_1 + 0.11w_2 + 0.13w_3 + 0.18w_4$  with standard deviation  $\sigma = \sqrt{0.02^2w_1^2 + 0.15^2w_2^2 + 0.15^2w_3^2 + 0.25^2w_4^2}$ .

Assume that as a function of return  $x$ , we have the following utility:

$$U(x) = \begin{cases} x, & \text{if } x \geq 0 \\ ax, & \text{if } x < 0. \end{cases}$$

for some  $a \geq 1$ . This says that if we earn money, our utility (happiness) equals our earnings, while if we lose money, our negative utility (suffering) is some multiple  $a$  of our monetary losses. The parameter  $a$  thus represents risk aversion.

By standard probability theory, our overall expected utility from the portfolio is

$$f = \int_{-\infty}^{\infty} U(x) \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/(2\sigma^2)} dx.$$

Use the constraint that our total investment is 1 to solve for  $w_4$  in terms of  $w_1, w_2$ , and  $w_3$ . Then write a function in Mathematica `f[w1_,w2_,w3_,a_]` for  $f$  in terms of  $w_1, w_2, w_3$ , and  $a$  (use

`NIntegrate` to compute the integral, and for simplicity change the limits from  $\pm\infty$  to  $\pm 0.5$ ; use colon-equals in defining `f` to ensure that Mathematica does not attempt to numerically integrate before you plug in  $w_1$ ,  $w_2$ ,  $w_3$ , and  $a$ ).

Use the `FindMinimum` command in Mathematica to maximize  $f$  (i.e., minimize  $-f$ ) for  $a = 1, 5, 25, 45$ . Discuss the results (it is OK if some  $w_j$  is negative; imagine that means you are selling existing investments of that type to buy other investments).

Investment # 2 is worse than investment # 3 (lower average return, same variability). Do you purchase # 2 in your optimal portfolio? Explain.