M368K
Homework #8

Burden and Faires.

Section 10.3 (#2b[1], 10b). Section 10.4 (#1b[2]). Section 10.5 (#1b[3], 2c[3]).

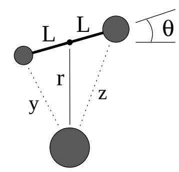
[1]Find $x^{(2)}$ given $x^{(0)} = (5, 2, 0)$.

[2]Find $x^{(1)}$ given $x^{(0)} = (1, 1.5)$; use $g(x) = ||F(x)||_2^2$ and $\alpha_0 = 1$.

[3]In each case, identify which of the two known solutions the continuation curve is approaching.

Programming mini-project.

Two molecules, where one is modeled as a single sphere and the other as a pair of spheres joined by a rigid link, bind to each other by adopting a configuration which minimizes an interaction energy between them. This energy describes how the two molecules are attracted to each other, but experience repulsion if they get too close. We suppose the interaction energy E is a function of the separation distance r and orientation angle θ,



$$E(r, \theta) = \left[\frac{a^2}{y^2} - \frac{2a}{y}\right] + \left[\frac{b^2}{z^2} - \frac{2b}{z}\right],$$

where $y = (L\cos\theta)^2 + (r - L\sin\theta)^2$, $z = (L\cos\theta)^2 + (r + L\sin\theta)^2$ and a, b and L are constants. Here we use the method of steepest descent to find configurations (r, θ) that minimize E. For concreteness, we assume $\{a, b, L\} = \{1.0, 1.5, 0.7\}$ in appropriate units.

(a) Download the C++ files `program8.cpp` and `descent.cpp` from the course webpage. Complete the function `descent.cpp` so that it implements the steepest descent method on a given function $g(x)$ with gradient $\nabla g(x)$.

(b) Consider the function $g(x) = E(r, \theta)$, where $x = (r, \theta)$, and find an expression for the gradient $\nabla g(x)$. Use steepest descent to find a minimum starting from at least three different choices of $x^{(0)}$. Assume the region of interest is $0 < r \leq 5$ and $-\pi \leq \theta \leq \pi$ and iterate until $||\nabla g(x^{(k)})||_2 < 10^{-6}$. Report the configuration (r, θ) and energy E for each minimum point you find. Do different choices of $x^{(0)}$ lead to genuinely different solutions, or do they all lead to a single solution up to the tolerance? [Note: E becomes infinite if the molecules get too close to each other, so you should avoid initial guesses with small r. Also, you should avoid large step sizes, so use $\alpha_0 = 0.2$.]

Turn in: completed copies of `descent.cpp` and `program8.cpp` and response to (b).