EECS 868: Homework 2
Due: Monday, February 24, 2020 (Hand-in via the EECS office by 12pm)

Important Directions: Please hand-in a hardcopy of all written exercises, Matlab codes, and Matlab output. Do not submit any portion of your homework electronically.

Linesearch Question:
1. Exercise 3.9 on p.64 in Nocedal and Wright.

Trust-Region Questions:
1. Exercise 4.2 on p.98 in Nocedal and Wright.
2. The solution to the trust region subproblem we have been studying is:
   \[ p(\mu) = -(B_k + \mu I)^{-1}\nabla f(x_k), \]
   for the unique \( \mu \geq 0 \) such that \( \|p(\mu)\| = \Delta_k \), unless \( \|p(0)\| \leq \Delta_k \), in which case \( p(0) = p_k^N \) is the solution. Now consider computing \( \mu \) such that \( \Phi(\mu) = \|p(\mu)\|_2 - \Delta_k = 0 \).
   (a) Derive Newton’s method for this problem and show that it underestimates the exact solution \( \mu^* \) for all \( \mu \geq 0, \Phi'(\mu) < 0, \Phi''(\mu) > 0 \).
   (b) As an alternative to Newton’s method, consider a one-dimensional version of \( \Phi(\mu) \) and consider a local model of the form
   \[ m_k(\mu) = \frac{\alpha_k}{\beta_k + \mu} - \Delta_k. \]
   (Note that \( \alpha_k, \beta_k \) are free parameters and do not represent our usual notation.) Determine \( \alpha_k, \beta_k \) such that \( m_k(\mu_k) = \Phi(\mu_k) \) and \( m_k'(\mu_k) = \Phi'(\mu_k) \). Once you have your model for \( m_k(\mu) \), choose \( \mu_+ \) such that \( m_k(\mu_+) = 0 \). Determine an expression for \( \mu_+ \) in terms of \( \mu_k \). Compare the steplengths of this technique with those of the Newton method for two cases: \( \mu_k < \mu_+ \) and \( \mu_k > \mu_+ \).

Application Question:
1. A simplified model for a cluster with \( N \) atoms is given by the Lennard-Jones potential, i.e.,
   \[ U(r) = 4\epsilon \sum_{i<j}^N \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \right], \]
   where \( \sigma \) and \( \epsilon \) are, respectively, the Lennard-Jones length and energy parameters, and \( r_{ij} \) is the distance between particles \( i \) and \( j \).
   (a) Using one of your Matlab codes for unconstrained optimization which you implemented for this assignment, simulate the behavior of a cluster of \( N = 5 \) atoms using the above model. First fix values of \( \epsilon \) and \( \sigma \) above. Then randomly generate a set of initial positions in 3D for the atoms. (Use the rand or randn in Matlab for this purpose. Type help followed by the name of the function to obtain a description of the method.) Run your unconstrained optimization code until an equilibrium configuration is obtained. Print the relative distances for the atoms in their final configuration. (Use fprintf to print the output. Type help fprintf to learn more.)
   (b) Repeat the above simulation several times using fixed \( \epsilon \) and \( \sigma \) but different starting configurations of the atoms. Do you obtain the same equilibrium condition each time?
   (c) Summarize your findings.