AMS 527, Spring 2014, Homework 2

100 points. Due: Monday 02/24

Electronic submission is required for the programming problems. Please email your programs and the report to the TA. Your email should have the subject line “AMS527 HW#2 Submission”. For the written part, you are encouraged (but not required) to typeset using \LaTeX or \TeX (an easy-to-use front-end of \LaTeX). For electronic submission, homework is due at 11:59pm on the due date. For paper submission, homework is due in class on the due date.

For this assignment, the programs can be written in MATLAB, C/C++, or Java.

1. (10 points) Exercise 5.5 on page 248 of the textbook.
   (a) Show that the iterative method
   \[ x_{k+1} = x_k - \frac{x_k f(x_k) - x_{k-1} f(x_{k-1})}{f(x_k) - f(x_{k-1})} \]
   is mathematically equivalent to the secant method for solving a scalar nonlinear equation \( f(x) = 0 \).
   (b) When implemented in finite-precision floating-point arithmetic, what advantages or disadvantages does the formula given in part (a) have compared with the formula for the secant method given in Section 5.5.4?

2. (10 points) Exercise 5.13 on page 249 of the textbook.
   Consider the system of equations
   \[
   \begin{align*}
   x_1 - 1 &= 0 \\
   x_1 x_2 - 1 &= 0
   \end{align*}
   \]
   For what starting point or points, if any, will Newton’s method for solving this system fail? Why?

3. (10 points) Exercise 5.14 on page 249 of the textbook.
   Supply the details of a proof that if \( x^* \) is a fixed point of the smooth function \( g : \mathbb{R} \rightarrow \mathbb{R} \), and \( g'(x^*) = 0 \), then the convergence rate of the fixed point iteration scheme \( x_{k+1} = g(x_k) \) is at least quadratic if started close enough to \( x^* \).

   Use the first and second order optimality conditions to show that \( x^* = [2.5, -1.5, -1]^T \) is a constrained local minimum for the function
   \[ f(x) = x_1^2 - 2x_1 + x_2^2 - x_3^2 + 4x_3 \]
   subject to
   \[ g(x) = x_1 - x_2 + 2x_3 - 2 = 0 \]

   Let \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) be given by
   \[ f(x) = \frac{1}{2} x^T A x - x^T b + c, \]
where $A$ is an $n \times n$ symmetric positive definite matrix, $b$ is a vector, and $c$ is a scalar.

(a) Show that Newton’s method for minimizing this function converges in one iteration from any starting point $x_0$.

(b) If the steepest descent method is used on this problem, what happens if the starting value $x_0$ is such that $x_0 - x^*$ is an eigenvector of $A$, where $x^*$ is the solution?

Prove that the block $2 \times 2$ Hessian matrix of the Lagrangian function for equality-constrained optimization (see Section 6.2.3) cannot be positive definite.

7. (20 points) Computer problem 5.20 on page 252 of the textbook. Submit your code and a report.
(a) According to quantum mechanics, the ground state of a particle in a spherical well is determined by the system of nonlinear equations

$$\frac{x}{\tan(x)} = -y, \quad x^2 + y^2 = s^2,$$

where $s$ depends on the mass and radius of the particle and the strength of potential. In appropriate units, $s = 3.5$. Use any method of your choice to solve this nonlinear system.

(b) The first excited state of the particle is determined by the nonlinear system

$$\frac{1}{x \tan(x)} - \frac{1}{x^2} = \frac{1}{y} + \frac{1}{y^2}, \quad x^2 + y^2 = s^2.$$

Again, use any method of your choice to solve this nonlinear system.

8. (20 points) Computer problem 6.9(a) and (b) on page 304 of Heath book. Submit your code and a report.
Write a program to find a minimum of Rosenbrock’s function,

$$f(x, y) = 100(y - x^2)^2 + (1 - x)^2$$

using each of the following methods:

(a) Steepest descent
(b) Newton

You should try each of the methods from each of the three starting points $[-1 \ 1]^T$, $[0 \ 1]^T$, and $[2 \ 1]^T$. For any line searches and linear system solutions required, you may use either library routines or routines of your own design. Plot the path taken in the plane by the approximate solutions for each method from each starting point.