Math 226A
Homework 3
Due Friday, November 17th

1. Suppose that $f(x_*) = f'(x_*) = 0$ and $f''(x_*) \neq 0$, and that f''' is continuous on an interval around x_*. Show that Newton's method converges and

$$\lim_{k \to \infty} \frac{e_{k+1}}{e_k} = \frac{1}{2},$$

where $e_k = |x_k - x_*|$.

2. Write a program to solve a system of equations using Newton's method with the option to include line searching. The program applies Netwton's method to find the solution to $f(x) = 0$, where $f : \mathbb{R}^n \to \mathbb{R}^n$. For simplicity use absolute tolerances on the size of the norm of $f(x_k)$ or the size of norm of $\delta x = x_{k+1} - x_k$ as the stopping criteria. You should also include a maximum number of iterations in case the iteration is failing to converge. Your program should take as input

   - A function for evaluating f at any value of x.
   - A function for evaluating the Jacobian of f at any value of x.
   - The initial guess, x_0.
   - Absolute tolerances for f and for δx.
   - The maximum number of iterations allowed.
   - A flag to choose whether line searching is performed.

   For each of the problems below and for each initial condition, run your code both with and without line searching. For each run, report the norm of f at each iteration, and discuss your results.

   (a) $f_1(x) = \dfrac{5 - 2x_1}{2x_2 - 3}$, $f_2(x) = \dfrac{5 - 2x_2}{2x_1 - 3}$,
   with $x_0 = (1, 1)$, $x_0 = (3, 3)$, $x_0 = (10, 10)$.

   (b) $f(x) = \dfrac{x^2}{1 + x^2}$, with $x_0 = 1$, $x_0 = 10$.

   (c) $f_1(x) = x_1 x_2 + x_1^3 + 4$, $f_2(x) = x_1 x_2^2 + x_2 + 6$, with $x_0 = (-1, -1)$, $x_0 = (1, 1)$.

3. In this problem, you use your Newton's method code from the previous problem to approximately solve a nonlinear PDE that has multiple solutions. By solving the time dependent problem

$$u_t = \epsilon u_{xx} - \exp(-|u|)u + g \quad \text{for } 0 \leq x \leq 1,$$
$$u(0, t) = u(1, t) = 0$$

to steady state for some parameters, you will find two different solutions depending on the initial condition. There is a steady state solution which is dynamically unstable, and thus does not arise from solving the time dependent problem numerically.

In this problem you solve for all three solutions to the boundary value problem

$$\epsilon u_{xx} - \exp(-|u|)u + g = 0,$$
$$u(0) = u(1) = 0.$$

Discretize the interval into the points $x_j = j\Delta x$ for $j = 0 \ldots N+1$ and $\Delta x = 1/(N+1)$. Let $u_j \approx u(x_j)$. For the approximation to the second derivative, use the standard 3-point, second-order discritzation

$$u_{xx}(x_j) \approx \frac{u_{j-1} - 2u_j + u_{j+1}}{\Delta x^2}.$$

The discretized problem is

$$A\vec{u} + F(\vec{u}) = 0,$$

where $\vec{u}_i \approx u(x_i)$ for $i = 1 \ldots N$ is a vector of approximate solution values on the interior, $F_i(\vec{u}) = -\exp(-|u_i|)u_i + g$, and A is the matrix

$$A = \frac{\epsilon}{\Delta x^2}\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}$$

(a) For the parameter values $\epsilon = 10^{-3}$ and $g = 0.25$, use your Newton's method code to find the two stable solutions first. We can find them by considering two different approximations.

- Consider u and u_{xx} small, and take the limit $\epsilon = 0$ to get a good initial guess for one solution.
- Consider u large, and thus $\exp(-|u|)$ is exponentially small, to get a good initial guess for the second solution.

(b) For the same parameter values, find the third solution by using initial guesses which are linear combinations of the two solutions found in the previous problem. Write a code that searches along linear combinations of the two solutions to find the third.

Plot the three different solutions you obtained.

4. (a) Write two programs to perform the (reduced) QR factorization using the classical Gram-Schmidt algorithm and the modified Gram-Schmidt algorithm. You will use these in the next part.

(b) Find an 11th degree polynomial that approximates the function $\cos(4x)$ evaluated at 50 equally spaced points on the interval $[0, 1]$ by solving a discrete least squares problem. Use the basis $\{1, x, \ldots, x^{11}\}$ for the polynomial so that the unknowns of the least squares problem are the 12 coefficients of

$$p(x) = a_0 + a_1 x + \ldots + a_{11}x^{11}.$$

The matrix that arises in the discrete problem is 50×12. Set up the linear least squares problem for the coefficients, and solve it using the methods below:

i. Form the normal equations and solve them.

ii. Use a QR factorization generated by classical Gram-Schmidt.

iii. Use a QR factorization generated by modified Gram-Schmidt.

iv. Use a QR factorization generated by Householder reflectors. You do not need to write the factorization code; you can use Matlab 's `qr` command, or something similar if you are using another language.

v. Use Matlab 's least squares solver by $A \backslash b$. This is also based on QR, but it includes pivoting for added stability.

For each method give the 2-norm of the residual, and estimate the error in the coefficients. Comment on how each method performed.

By solving the problem in quad precision arithmetic, I obtained a residual with norm `7.999154576455076e-09`, with coefficients given in the table below.

a_0	1.000000000996606e+00
a_1	-4.227430949815150e-07
a_2	-7.999981235683346e+00
a_3	-3.187632625738558e-04
a_4	1.066943079610163e+01
a_5	-1.382028878048870e-02
a_6	-5.647075625417684e+00
a_7	-7.531602738192263e-02
a_8	1.693606966623459e+00
a_9	6.032106743884792e-03
a_{10}	-3.742417027133638e-01
a_{11}	8.804057595513443e-02

(c) To help understand the differences in the three QR factorizations (classical GS, modfied GS, Householder) from the previous problem, examine the norm of $Q^T Q - I$. What should this be? How does it differ between the different algorithms? Explain the difference in results.