Introduction to Scientific Computing with Fortran 90
Project II

Due: Monday, 2/15

The goal of this project is to complete our module and corresponding driver program to incorporate the methods we discussed for finding a root of $f(x) = 0$.

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1. You should already have function routines for Newton's method, the bisection method and regula falsi. Add function routines to your module to implement the Secant Method and Fixed Point Iteration. Compile this.

2. Modify your driver program to include the options to perform all 5 methods. Modify your code so that it writes pertinent information to file; include method used, iteration number, approximation, the residual, and the difference in successive iterates.

3. Run each of your codes to find the root of $f(x) = x^2 - 4\sin(x)$ in the interval $[1, 3]$. For the fixed point iteration choose $g(x) = 2\sqrt{\sin x}$. Choose your initial guess(es) in this interval. Choose a tolerance of 10^{-5}. Turn in the final version of your module and main program as well as either a print out of your files containing the output or the text or pdf file itself.

4. Now we want to run the code for a problem we know the exact root so that we can compute a numerical rate of convergence. Consider the polynomial $f(x) = (x - 2)(-x^5 - 0.5)$ which has a root at $x = 2$. Use the initial guess of 1 for Newton's method, 1.75, 3 for Secant Method and 1,3 for Bisection Method. Make a table of your iteration number, the approximation, the error $|2 - x^k|$, and the numerical rate of convergence. Compare your rates of convergence. Turn in this output.

5. (grads only) There is a method, sometimes called Brent's Method, which also requires bracketing the root but has faster convergence than the Bisection or Regula Falsi methods. Below is the description of the method. Implement this method into your module and estimate the numerical rate of convergence.

Step 1 Select x^0, x^2 so that $f(x^0)f(x^2) < 0$

Step 2 Bisect $[x^0, x^2]$ to obtain x^1 and a third point $(x^1, f(x^1))$

for $k = 2, 3, \ldots$

Step 3 The new iterate x^{k+1} is obtained by fitting a quadratic polynomial through the three points $(x^i, f(x^i))$, $i = k-2, k-1, k$ and setting it equal to the point where this quadratic crosses the x axis.

Step 4 Check for convergence; if converged, print out results and stop. Otherwise select from these four x-points (x^{k+1}, x^k, x^{k-1} and x^{k-2}) three which bracket the root and lie closest together. (These three points become the new x^i, $i = k-2, k-1, k$ and I relabel them so that they read from left to right.)

Step 5 Go to STEP 3

If you fit a quadratic, $ax^2 + bx + c$ with the three points (x_0, x_1, x_2) and corresponding y values (y_0, y_1, y_2) and find where this quadratic passes through the point $(x_3, 0)$ you get the formula

$$x_3 = \frac{y_1 y_2 x_0}{(y_0 - y_1)(y_0 - y_2)} + \frac{y_0 y_2 x_1}{(y_1 - y_0)(y_1 - y_2)} + \frac{y_0 y_1 x_2}{(y_2 - y_0)(y_2 - y_1)}$$