C for Science - 2011 - Practical Exercise #5

The Newton-Raphson method can be used to compute the root of function which we know the derivative of. Given $F(x)$ we find x^* such that $F(x^*) = 0$. The algorithm starts with an initial guess, x_0, for the root and calculated an improved guess from the formula:

$$x_{n+1} = x_n - \frac{F(x_n)}{F'(x_n)}, \quad n = 0, 1, \ldots \tag{1}$$

Iteration stops when a *termination criterion* is met, some common ones include:

- A maximum number of iterations has been reached (we don't want to wait forever!).
- $F(x_n)$ is "close" to zero.
- $|x_{n+1} - x_n|$ is "small".

(also note that we really need $F'(x_n) \neq 0$).

1. Place the following at the top of your program:

   ```
   typedef double (* fx)(double x);
   ```

   (this is a function pointer to a function which takes in one `double` and returns one `double`).

2. Write a C function to carry out Newton iteration following the prototype:

   ```
   int Newton(double * x, fx f, fx df, int max_its, double tol);
   ```

   where,

   - `f` is the $F(x)$ function we are trying to solve.
   - `df` corresponds to the derivative of the target function, i.e. $F'(x)$.
   - `max_its` is the maximum number of iterations that are allowed.
   - `tol` is the algorithm *tolerance*, if either $|F(x_n)| <$ `tol` or $|x_{n+1} - x_n| <$ `tol`, iteration should stop.
   - `x` is a pointer to an initial guess, when the Newton iteration has finished, this should be set to x_{n+1}.
   - `Newton` should `return` the number of iterations carried out.

3. Write a `main` function to

   (a) prompt the user for an initial guess, maximum number of iterations and a tolerance.

   (b) Call the `Newton` function to compute the answer.

   (c) Print out: x_{n+1} and $F(x_{n+1})$.

4. Test the program with the case $F(x) = x^2 - 2$ at first, with an initial guess of $x_0 = 1$:

   (a) What is the lowest tolerance setting you can use before the method fails to converge (using fewer than 10 iterations)?

5. Test your solver on the Bessel function (present in GSL and other libraries). Take $F(x) = J_0(x)$, $F'(x) = -J_1(x)$ and try an $x_0 = 2$.