

Queens College, CUNY, Department of Computer Science
Numerical Methods
CSCI 361 / 761
Spring 2018
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due Friday July 13, 2018 11.59 pm

2 Homework set 2

- Please email your solution, as a file attachment, to `Sateesh.Mane@qc.cuny.edu`.
- Please submit one zip archive with all your files in it.
 1. The zip archive should have either of the names (CS361 or CS761):
`StudentId_first_last_CS361_hw2.zip`
`StudentId_first_last_CS761_hw2.zip`
 2. The archive should contain one “text file” named “hw2.[txt/docx/pdf]” and one cpp file per question named “Q1.cpp” and “Q2.cpp” etc.
 3. Note that not all homework assignments may require a text file.
 4. Note that not all questions may require a cpp file.
- Experience has demonstrated that in many cases the source of difficulty is not the mathematics.
- The source of difficulty is the English (understanding the text).
- If you do not understand the words in the lectures or homework, **THEN ASK**.
- If you do not understand the concepts in the lectures or homework, **THEN ASK**.
- Send me an email, explain what you do not understand.
- Do not just keep quiet and then produce nonsense in exams.

2.1 Functions

- We shall write code to implement the bisection and Newton–Raphson root finding algorithms.
- For bisection, we require only the function value.
- For Newton–Raphson, we also require the derivative.
- **Write the following forward declarations, which we shall use below.**

```
double func(double x);  
void func(double x, double &f, double &fprime);
```

2.2 Bisection

- The function signature for our bisection function is

```
int root_bisection(double target, double tol_f, double tol_x, int max_iter,  
                  double x_low, double x_high,  
                  double & x, int & num_iter)
```

- The return type is “int” not void, because the algorithm might not converge. If the calculation succeeds, we return 0. If it fails, we return 1.
- The inputs are (i) double target, (ii) double tol_f, (iii) double tol_x, (iv) int max_iter, (v) double x_low, (vi) double x_high.
- The outputs are (vii) double & x (the root), (viii) int & num_iter (number of iterations).
- Obviously target is the target value. We wish to solve $f(x) = \text{target}$.
- We also need tolerance parameters.
Remember that an iterative algorithm needs a cutoff parameter to stop iterating.
We use tol_f for convergence along the y -axis and tol_x for convergence along the x -axis.
- As a safety check, we also input an upper limit max_iter on the number of iterations, in case the computations take too long.

The following pseudocode describes the steps. You can use it as the basis to write a working function.

1. Initialize $x = 0$ and $\text{num_iter} = 0$.
2. Calculate a value $\text{double } y_{\text{low}} = \text{func}(x_{\text{low}})$.
Also calculate $\text{double } \text{diff_y_low} = y_{\text{low}} - \text{target}$.
3. If $|\text{diff_y_low}| \leq \text{tol_f}$, then we are done.
The value of y_{low} is already within the tolerance.
Set $x = x_{\text{low}}$ and “return 0” (= success) and exit.
4. Next calculate a value $\text{double } y_{\text{high}} = \text{func}(x_{\text{high}})$.
Also calculate $\text{double } \text{diff_y_high} = y_{\text{high}} - \text{target}$.
5. If $|\text{diff_y_high}| \leq \text{tol_f}$, then we are done.
The value of y_{high} is already within the tolerance.
Set $x = x_{\text{high}}$ and “return 0” (= success) and exit.
6. Next we must check if we have bracketed a root.
In order to bracket a root, y_{low} and y_{high} must lie on opposite sides of target.
This means diff_y_low and diff_y_high must have **opposite signs**.
7. Test if $(\text{diff_y_low} * \text{diff_y_high} > 0.0)$.
If yes, **then we have failed**. The inputs x_{low} and x_{high} do not bracket a root.
Set $x = 0$ and **“return 1” (= fail)** and exit.

8. If we have made it this far, then we know that we have bracketed a root.
We know that there is a solution for x somewhere between `x_low` and `x_high`.

9. Hence we begin the bisection (iteration) loop.

```
for (num_iter = 1; num_iter < max_iter; ++num_iter) {  
    // (to be filled in below)  
}
```

10. In the loop, set `x = (x_low + x_high)/2.0` and calculate `double y = func(x)`.

11. Also calculate `double diff_y = y - target`.

12. If `|diff_y| ≤ tol_f`, then we are done.

The value of `y` is within the tolerance.

We have found a “good enough” value for x .

Hence “return 0” (= success) and exit.

13. **Next test if `(diff_y * diff_y_low > 0.0)`.**

If yes, it means `y` and `y_low` are on the same side of `target`.

This means `x` and `x_low` are on the same side of the root.

Update `x_low = x`.

14. Else obviously `y` and `y_high` are on the same side of `target`.

Hence `x` and `x_high` are on the same side of the root.

Update `x_high = x`.

15. *Don't be in rush to iterate!* **There is one more test!**

16. We have tested for convergence in y , now we must test for convergence in x .

17. If `|x_high - x_low| ≤ tol_x`, then the algorithm has converged (up to the tolerance).

Note that the **tolerance is `tol_x`** in this test (convergence in x).

Hence “return 0” (= success) and exit.

18. If we have come this far, continue with the iteration loop.

19. If we exit the iteration loop after `max_iter` steps and the calculation still has not converged, then set $x = 0$ and `num_iter = max_iter` and “return 1” (= fail) and exit.

20. We have reached the end of the function. By now either we have a “good enough” answer (“return 0” = success) or not (“return 1” = fail).

2.3 Testing of function

- You will have to write a main program to call and test your function.
- However, you also need an actual example of a function $f(x)$.
- One simple example is a parabola.

```
double func(double x)
{
    return x*x;
}
```

- For later use with Newton–Raphson, also write the following function.

```
void func(double x, double &f, double &fprime)
{
    f = x*x;
    fprime = 2.0*x;
}
```

- The equation is therefore $f(x) = \text{target}$. The solution is $x = \pm\sqrt{\text{target}}$.
- Try `target = 4.0`. If your function works correctly, it should output $x = 2.0$ or -2.0 .
- Set `tol_f = tol_x = 1.0e-6` and `max_iter=100`.
- If `x_low=0.0` and `x_high=5.0`, the algorithm should converge to $x = 2.0$.
- If `x_low=-5.0` and `x_high=5.0`, the algorithm should return 1 and fail.
- You can devise other tests. Use your imagination.
- Try `x_low=-10.0` and `x_high=0.0`. Try `target =-1.0`.

2.4 Newton–Raphson

- Next let us write a function to implement the Newton–Raphson algorithm.
This function is in fact shorter than the one for bisection.

- The function signature for our Newton–Raphson function is

```
int root_NR(double target, double tol_f, double tol_x, int max_iter, double x0,  
            double & x, int & num_iter);
```

- The return type is “int” not void, because the algorithm might not converge.
If the calculation succeeds, we return 0. If it fails, we return 1.
- The inputs are (i) double `target`, (ii) double `tol_f`, (iii) double `tol_x`, (iv) int `max_iter`, (v) double `x0` (initial iterate).
- The outputs are (vi) double & `x` (the root), (vii) int & `num_iter` (number of iterations).
- Obviously `target` is the target value. We wish to solve $f(x) = \text{target}$.
- We also need tolerance parameters.
Remember that an iterative algorithm needs a cutoff parameter to stop iterating.
We use `tol_f` for convergence along the y -axis and `tol_x` for convergence along the x -axis.
- As a safety check, we also input an upper limit `max_iter` on the number of iterations, in case the computations take too long.

The following pseudocode describes the steps. You can use it as the basis to write a working function.

1. Declare some useful variables at the start of the function.

```
const double tol_fprime = 1.0e-12;  
double f = 0;  
double fprime = 0;
```

2. The const parameter “tol_fprime” is to guard against division by zero.
The value of 1.0e-12 is arbitrary.
3. We do not need any preliminary tests.
Set `x = x0` (= initial iterate) and begin the main iteration loop.

```
x = x0;  
for (num_iter = 1; num_iter < max_iter; ++num_iter) {  
    // (to be filled in below)  
}
```

4. We could begin with `num_iter = 0` but this is not important.

5. In the loop, call `func(x,f,fprime)`.
6. Also calculate `double diff_f = f - target`.
7. If $|\text{diff_f}| \leq \text{tol_f}$, then we are done.
The value of `f` is within the tolerance.
We have found a “good enough” value for x .
Hence “return 0” (= success) and exit.
8. Next test if $|\text{f_prime}| \leq \text{tol_fprime}$.
If yes, then this will cause a division by zero and *the Newton–Raphson iteration fails*.
Set `x = 0` and “return 1” (= fail) and exit.
9. Calculate `double delta_x = diff_f/fprime`.
10. Now test for convergence in x .
11. If $|\text{delta_x}| \leq \text{tol_x}$, then the algorithm has converged (up to the tolerance).
Note that the **tolerance is `tol_x`** in this test (convergence in x).
Hence “return 0” (= success) and exit.
12. If the convergence tests have not passed, update the value of x (note the minus sign).

`x -= delta_x;`
13. Continue with the iteration loop.
14. If we exit the iteration loop after `max_iter` steps and the calculation still has not converged, then set $x = 0$ and `num_iter = max_iter` and “return 1” (= fail) and exit.
15. We have reached the end of the function. By now either we have a “good enough” answer (“return 0” = success) or not (“return 1” = fail).
16. Probably the best test is to use the same main program that you wrote to call the bisection algorithm and use it to also call the Newton–Raphson function. Give the same target and tolerance parameters to both functions. For bisection you have to input `x_low` and `x_high` whereas for Newton–Raphson you have to input a starting oterate `x0`. If they both converge, the output value of x should be the same in both cases (up to the tolerance). Also print out the number of iterations `num_iter` from both function calls. In general, Newton–Raphson should converge (much) more quickly.

2.5 Cumulative Normal Distribution

- A more interesting function is the **cumulative normal distribution**.
- The probability density function for the normal probability distribution is (with mean = 0 and variance = 1)

$$p(x) = \frac{e^{-x^2/2}}{\sqrt{2\pi}} \quad (-\infty < x < \infty). \quad (2.5.1)$$

- The **cumulative normal distribution** is defined via the integral

$$N(x) = \int_{-\infty}^x \frac{e^{-t^2/2}}{\sqrt{2\pi}} dt \quad (-\infty < x < \infty). \quad (2.5.2)$$

- The difficulty is, how do we compute $N(x)$ for arbitrary values of x ?
The above formula is an integral, which by itself is complicated to compute.
- Fortunately C++ (also Excel/Visual Basic) and other languages have a function $\text{erf}(x)$.
It is known as the “error function” (hence “erf”) as is defined as

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt. \quad (2.5.3)$$

- Hence we obtain $N(x)$ via

$$N(x) = \frac{1 + \text{erf}(x/\sqrt{2})}{2}. \quad (2.5.4)$$

- **The following functions will serve our needs.**

```
double cum_norm(double x)
{
    const double root = sqrt(0.5);
    return 0.5*(1.0 + erf(x*root));
}
double func(double x)
{
    return cum_norm(x);
}
void func(double x, double &f, double &fprime)
{
    const double pi = 4.0*atan2(1.0,1.0);
    f = cum_norm(x);
    fprime = exp(-0.5*x*x)/sqrt(2.0*pi);
}
```

- Use this and run some tests with both bisection and Newton–Raphson.
Unlike a quadratic, it is not simple to solve the equation $N(x) = \text{target}$.
By construction, $N(-\infty) = 0$ and $N(\infty) = 1$ and for finite values of x , then $0 < N(x) < 1$.
Hence to obtain convergence, the target value must lie in the range $0 < \text{target} < 1$.

2.6 Multiple test functions

- **Write only one bisection function and one Newton–Raphson function.**
- Do not write `root_bisection_quadratic()` and `root_bisection_cum_norm()`, etc.
- Also do not write a new cpp file every time you write a new test function.
- Although this will work for a homework assignment, in a real software library function we cannot write a new function or new file for each new test function. What will happen if the client wants to use $f(x) = x^3$ and solve $x^3 = \text{target}$? Or some other function?
- A real software library root-finding function would take an extra input argument for a function pointer. I decided this is too complicated and too much programming burden on you. A lot of programming formalism, which has nothing to do with the subject matter of this course.
- *What to do?*
- Use `#ifdef` preprocessor directives. Here is a sample code of what I mean. It is not pretty but it works. I added a third selection “cubic” for $f(x) = x^3$ to illustrate the basic idea. Uncomment one of the `#define` statements to select a test function.
- Then `root_bisection()` etc. calls only `func()` and not a different function for each test case.
- It is true that you must recompile the program every time you change the choice of test function. It is not a pretty solution, but it works.

2.6.1 Preprocessor code

uncomment one of the #define choices below to select a test function

```
//#define func_quadratic
//#define func_cubic
#define func_cum_norm

#ifdef func_quadratic
double func(double x){
    return x*x;
};
void func(double x, double &f, double &fprime){
    f=x*x;
    fprime=2.0*x;
};
#endif // func_quadratic

#ifdef func_cubic
double func(double x){
    return x*x*x;
};
void func(double x, double &f, double &fprime){
    f=x*x*x;
    fprime=3.0*x*x;
};
#endif // func_cubic

#ifdef func_cum_norm
double cum_norm(double x)
{
    const double root = sqrt(0.5);
    return 0.5*(1.0 + erf(x*root));
}
double func(double x)
{
    return cum_norm(x);
}
void func(double x, double &f, double &fprime)
{
    const double pi = 4.0*atan2(1.0,1.0);
    f = cum_norm(x);
    fprime = exp(-0.5*x*x)/sqrt(2.0*pi);
}
#endif // func_cum_norm
```

2.6.2 Main program pseudocode

```
// header files etc

int main()
{
    // set inputs
    // call root_bisection(...)
    // call root_NR(...)
    // check if the results from bisection and NR match (up to tolerance)

    // CALL THE TEST FUNCTION USING X = ROOT (bisec and NR roots)
    // IS THE VALUE F(X_ROOT) CLOSE TO ZERO?

    // in other words, did the algorithm converge correctly?

    return 0;
}
```