LOCATING ROOTS FOR NONLINEAR EQUATIONS

KEY WORDS. nonlinear equations, iterative method, bisection method, Newton's method, secant method.

GOAL.

- Introduce nonlinear equation.
- Learn about iterative methods for solving nonlinear equations

1 A Practical Problem: Floating Spherical Ball.

According to Archimedes, if a solid that is lighter than a fluid is placed in the fluid, the solid will be immersed to such a depth that the weight of the solid is equal to the weight of the displaced fluid. For example, a spherical ball of unit radius will float in water at a depth H (which is the distance from the bottom of the ball to the water line) determined by the density of the ball ρ_b, assuming that the density of the water $\rho_w = 1$. The volume of the submerged segment of the sphere is

$$V = \int_0^H \pi r^2(h) dh = \int_0^H \pi(1-(1-h)^2)dh = (H^2 - \frac{H^3}{3}) \tag{1}$$

To find the depth at which the ball floats, we must solve the equation that states that the water density times the volume of the submerged segment is equal to the ball density ρ_b times the volume of the entire sphere, i.e.,

$$\rho_w \times V = \rho_b \times \frac{4\pi}{3}, \tag{2}$$

which simplifies to

$$H^3 - 3H^2 + 4\rho_b = 0 \tag{3}$$

The depth H of physical interest lies between 0 and 2 since the ball is of unit radius and H is measured upwards from the bottom of the ball. The question here is how to find this depth H.

Exercise 1.1. Assume that $\rho_b = 1/3$, by using the Intermedia Value Theorem, show that there exists a root H_0, s.t. $H_0^3 - 3H_0^2 + 4\rho_b = 0$.

2 Math Problem: Finding Roots

Definition 2.1. Let f be a real or complex valued function of a real or complex variable. A number r, real or complex, for which

$$f(r) = 0 \tag{4}$$

is called a root of that equation or a zero of the function f .

For example, the function $f(x) = 2x - 4$ has the zero $r = 2$. The function $g(x) = x^2 - 3x + 2$ has two roots $r = 1, 2$. For our floating sphere problem, the function f is given by $f(H) = H^3 - 3H^2 + 4\rho_b$. Thus, our floating sphere problem is an example of the general root finding problem.

Another typical root finding problem is the problem of finding the points of intersection of two curves. Let $y = f(x)$ and $y = g(x)$ be two continuous real-valued functions. Geometrically, each function is a curve in the (x, y) plane. We wish to find a point of intersection of these two curves. In other words, we need to find an r such that

$$f(r) = g(r), \tag{5}$$

or

$$f(r) - g(r) = 0. \tag{6}$$

Therefore, a point of intersection of the curves $y = f(x)$ and $y = g(x)$ is a zero of the function $h(x) = f(x) - g(x)$.

A first and natural question to ask about locating roots for nonlinear equations is

- Does there ever exist a root?
- If yes, how many roots does the equation have?

The following Intermediate-Value Theorem only partially answers the questions.

Theorem 2.2. *(Intermediate-Value Theorem) Let $f(x)$ be a continuous function on a close interval $[a, b]$. If*

$$f(a)f(b) < 0, \tag{7}$$

then there exists an $r \in (a, b)$, s.t. $f(r) = 0$.

Remark 2.3. In general, the existence and the number of roots for nonlinear equations is an open question. The Intermedia-Value Theorem is a sufficient condition for the existence of a root, but not necessary condition.

Exercise 2.4. Could you think of an example, when the assumption of Intermedia-Value Theorem is not satisfied, but the existence of root is still valid?

3 Numerical Approach: Iterative Methods

In this section, we discuss some iterative methods that can be applied to locate roots of nonlinear equations. Iterative methods proceed by producing a sequence of numbers that (hopefully) converges to a root of interest. The implementation of any iterative technique requires that we deal with the following issues:

- Where do we start the iteration (how do we choose an initial guess)? How do we design the iteration procedure?
- How do we know when to terminate the iteration?
- Does the scheme converge? If so, how fast?

Example 3.1. (Iterative scheme for calculating square root of m) We wish to find the square root of any positive real number m. This question can be formulated as a root nding problem as follows:

- let $x = \sqrt{m}$.
- Take the square of both sides: $x^2 = m$.
- Move m to the left-hand side: $x^2 - m = 0$.

How do we design an algorithm to approximate $\sqrt{m}$? Let x_n be the current approximation to $\sqrt{m}$. A related approximation would be

$$x_n^* = \frac{m}{x_n}, \tag{8}$$

since $x_n \cdot x_n^* = m$. Also due to the fact that $x_n \cdot x_n^* = m$, it is not clear which one of x_n and x_n^* will do a better job in approximating $\sqrt{m}$. A compromise is the average of x_n and x_n^*. In other words, we take

$$x_{n+1} = \frac{1}{2}(x_n + \frac{m}{x_n}), \tag{9}$$

as the new approximation. With x_0 chosen appropriately, the relation (37) is an example of an iterative scheme.

Exercise 3.2. For m=3 and $x_0 = 1$, what are x_1, x_2, x_3?

3.1 Bisection Method

3.1.1 Description of the method

Suppose f is a continuous function that changes sign on the interval $[a, b]$. Then it follows from the Intermediate Value Theorem that f must have at least one zero in the interval $[a, b]$. This fact can be used to produce a sequence of even smaller intervals that each bracket a zero of f . Specically, assume that

$$f(a)f(b) < 0 \tag{10}$$

Then the function $y = f(x)$ must intersect the x-axis. In other words, there must be a point $r \in [a, b]$ such that $f(r) = 0$. Which point of $[a, b]$ is the root? A good guess would be the mid-point $c_0 = (a+b)/2$. With this guess, we compute the value of f at the mid-point c_0. There are two possible cases:

- $f(c_0) = 0$: This is fortuitous - we have found the zero, namely, c_0.
- $f(c_0) \neq 0$: In this case, we must have either $f(a)f(c_0) < 0$ or $f(c_0)f(b) < 0$.

In the second case, we conclude that there must be a zero in either $[a, c_0]$ or $[c_0, b]$. In either case, we are left with a half-sized bracketing interval. We repeat the same procedure to come up with an even smaller interval that brackets a zero of f , and denote by c_1 the mid-point of this new subinterval. Repeated use of this procedure will produce a sequence of approximations

$$c_0, c_1, c_2, \cdots \tag{11}$$

which converges to a zero of the function f; that is,

$$\lim_{n \to \infty} c_n = r \tag{12}$$

The following is a segment of MATLAB code that implements the bisection method in which the halving process can continue until the current interval is shorter than a designated positive tolerance `delta`.

```
  function root=BisectionM(f, a, b, delta, nmax)
  fa = f(a);
  fb = f(b);
  if fa*fb > 0
     disp('Initial interval does not bracket a root')
     return
  end
  itcount=0;
  while (abs(b-a) > delta & itcount<nmax)
    itcount=itcount+1;
    c=(a+b)/2;
    fc=f(c);
    if fa*fc<=0
% There is a root in the interval [a,c]
    b=c;
    fb=fc;
% Otherwise, there is a root in the interval [c,b]
    else
    a=c;
    fa=fc;
   end
```

```
end
root=(a+b)/2;
disp(sprintf('itcount = %i',itcount))
```

EXAMPLE 1. Find the largest root of

$$f(x) \equiv x^6 - x - 1 = 0$$

accurate to within `delta` $= 0.001$ using no more than 15 iterations. Please check that this root lies in the interval $[1, 2]$. Then we may choose $a = 1$ and $b = 2$, and obtain the following.

```
>> f=inline('x^6-x-1')

f =

     Inline function:
     f(x) = x^6-x-1

>> root = BisectionM(f,1.,2.,0.001,15)
itcount = 10

root =

    1.1343
```

It should be noted that the time required by a root-finder like *BisectionM()* is proportional to the number of function evaluations. The arithmetic that takes place outside of the function evaluations is typically insignificant.

Exercise 3.3. Use *BisectionM()* or your own code to solve the floating sphere problem (3) in which the sphere's density is 1/3.

3.1.2 The convergence of the bisection method

Consider the bracket $[a_n, b_n]$ at the iterative step n. Since $[a_n, b_n]$ was obtained from $[a_{n-1}, b_{n-1}]$ by the halving procedure, then with $c_n = (a_n + b_n)/2$ we have

$$|c_n - r| \le \frac{1}{2}|b_n - a_n| = \frac{1}{4}|b_{n-1} - a_{n-1}| = \cdots = \frac{1}{2^{n+1}}(b - a), \qquad (13)$$

where $(b-a)$ is the length of initial interval and r is one of the roots bracketed in $[a_n, b_n]$. In summary, if the bisection method is applied to a continuous function f on an interval $[a, b]$, where $f(a)f(b) < 0$, then, after n steps, an approximate root will have been computed with error at most $\frac{1}{2^{n+1}}(b - a)$.

Estimate (13) is an example of linear convergence of iterative methods. A sequence $\{x_n\}$ is said to converge linearly to a limit r if there is a constant C in the interval $[0, 1)$ such that

$$|x_{n+1} - r| \leq C|x_n - r|, \tag{14}$$

for $n > 0$. Then

$$|x_{n+1} - r| \leq C|x_n - r| \leq \cdots \leq C^{n+1}|x_0 - r|. \tag{15}$$

Thus it is a consequence of linear convergence that

$$|x_n - r| \leq AC^n, \quad C \in (0, 1] \tag{16}$$

The sequence produced by the bisection method obeys (16) as we see from (13).

A disadvantage of the bisection method is that it applies only to functions of one variable. Also, there are cases where the method is not applicable. (Please provide an example of such a case.)

3.2 Newton's Method

Newtons method is a procedure that approximates the zeros of a function f by a sequence of linearizations, and takes the form

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \tag{17}$$

for $n = 0, 1, 2, \cdots$ Here x_0 is an initial guess that must be chosen carefully to ensure convergence of the iterative scheme eq. (17).

3.2.1 Geometric derivation of Newton's method

Our objective is to approximate r which satisfies $f(r) = 0$. Graphically, the roots of the function $f(x) = 0$ are points of intersection of the curve $y = f(x)$ with the $x-$axis. Let x_n be an approximation to r at step n. We wish to update x_n with a better approximation called x_{n+1}. A geometric approach to determining x_{n+1} is given as follows:

- Draw the tangent line of the curve $y = f(x)$ at the point $(x_n, f(x_n))$. The slope of the tangent line at point $(x_n, f(x_n))$ is $f'(x_n)$. The equation of a straight line, passing by the point $(x_n, f(x_n))$ with slope $f'(x_n)$ is

$$y = f(x_n) + f'(x_n)(x - x_n) \tag{18}$$

- Find the intersection of the tangent line with the $x-$axis. This point of intersection is chosen as the new approximation x_{n+1}. To find the intersection of the tangent line with the $x-$axis, we set $y = 0$ in equation (18) and solve for x. This leads to

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \tag{19}$$

Exercise 3.4. Please draw a picture to illustrate Newton's method. Be sure to carefully label your picture.

3.2.2 Algebraic derivation of Newton's method

Newtons method can also be derived in the following way using the Taylor series of a function of one variable. Let x_n be the current approximation to a zero r of the function $f(x)$. The error, denoted by h, is given by

$$h = r - x_n, \tag{20}$$

from which it follows that

$$r = x_n + h. \tag{21}$$

Since r is a zero of $f(x)$, we have

$$f(x_n + h) = 0.$$

Using Taylor series at x_n, we arrive at the following,

$$f(x_n) + hf'(x_n) + \frac{h^2}{2!}f''(x_n) + \mathcal{O}(h^3) = 0. \tag{22}$$

If equation (22) is viewed as an equation in terms of the variable h, by solving for h from this equation we would obtain a true root of the function f. Unfortunately, this is impossible in practice. Therefore, we take only the first two terms of the series, which yields a linear equation to solve for h. This linear equation is

$$f(x_n) + hf'(x_n) = 0, \tag{23}$$

with solution

$$h = -\frac{f(x_n)}{f'(x_n)}. \tag{24}$$

Since we truncated the series in h, this is generally different from the true solution. However, the corrected solution

$$x_{n+1} = x_n + h = x_n - \frac{f(x_n)}{f'(x_n)} \tag{25}$$

provides a better approximation to the solution of $f(x) = 0$. This is the Newton's method.

3.2.3 Finding the $\sqrt{2}$ by Newton's method

Recall that the problem of finding the square root of 2 can be expressed as a solution of

$$x^2 - 2 = 0, \tag{26}$$

which is equivalent of locating zeros of $f(x) = x^2 - 2$. Since $f'(x) = 2x$, the Newton's method is given by

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{x_n^2 - 2}{2x_n} = \frac{1}{2}(x_n + \frac{2}{x_n}), \tag{27}$$

which is equation (37).

The following is a segment of MATLAB code that implements the Newton's method in which the iterative process can continue until the two successive approximations are close enough (tolerance `delta`).

```
function root=NewtonM(f, fderiv, x0, delta, nmax)
error =1;
itcount=0;
while abs(error) > delta & itcount<nmax
  fx=f(x0);
  dfx=fderiv(x0);
  if dfx == 0;
    disp('The derivative is zero. Stop.')
    return
  end
  x1=x0-fx/dfx;
  error = x1-x0;
  x0=x1;
  itcount=itcount+1;
end
if itcount >=nmax
disp('Maximum number of iterations exceeded')
root=x1;
else
disp(sprintf('itcount = %i',itcount))
root=x1;
end
```

Using the initial guess $x0$ as the starting point, we carry out a maximum of `nmax` iterations of Newton's method. Procedures must be supplied for the external functions f and f'. The parameter `delta` is used to control the convergence and is related to the accuracy desired or to the machine precision available.

EXAMPLE 2. Solve the problem in Example 1 using Newton's method with $x_0 = 1$.

```
>> f=inline('x^6-x-1')

f =
```

```
     Inline function:
     f(x) = x^6-x-1

>> fder=inline('6*x^5-1')

fder =

     Inline function:
     fder(x) = 6*x^5-1

>> root = NewtonM(f,fder,1.,0.001,6)
itcount = 4

root =

    1.1347

>> root = NewtonM(f,fder,1.,0.001,3)
Maximum number of iterations exceeded

root =

    1.1349
```

Exercise 3.5. Using Newton's method, solve the floating sphere problem (3) in which the sphere's density is 1/3. Be sure to clearly indicate your choice of initial guess(es). Compare your results with those obtained using the bisection method.

3.2.4 Convergence of Newton's method

To study the convergence of Newtons method, we derive a recursive relation for the error $e_n = r - x_n$. From Newtons method, by subtracting both sides of equation (17) from r, we obtain

$$e_{n+1} = e_n + \frac{f(x_n)}{f'(x_n)} = \frac{e_n f'(x_n) + f(x_n)}{f'(x_n)}. \tag{28}$$

It following from Taylor's Theorem that

$$f(r) = f(x_n) + (r - x_n)f'(x_n) + \frac{1}{2}(r - x_n)^2 f''(\xi_n), \tag{29}$$

with ξ_n lies between x_n and r. Since $f(r) = 0$, we have

$$f(x_n) + e_n f'(x_n) = -\frac{1}{2}e_n^2 f''(\xi_n). \tag{30}$$

Combining equation (28) and (30) gives,

$$e_{n+1} = -\frac{1}{2}e_n^2\frac{f''(\xi_n)}{f'(x_n)} \tag{31}$$

Assume that $f'(r) \neq 0$, that is, r is a simple zero of f . Then, there exists a neighborhood of r in which f' is nonzero. In other words, there exists a $\delta_0 > 0$ such that

$$|f'(x)| \geq c_0 > 0, \quad \text{whenever} \quad |x - r| \leq \delta_0. \tag{32}$$

Also assume that the second order derivative is bounded in this δ_0 neighborhood. Thus there is a constant M such that

$$|\frac{1}{2}\frac{f''(\eta)}{f'(x)}| \leq M, \tag{33}$$

for any η, $x \in (r - \delta_0, r + \delta_0)$. Thus from this bound and equation (31), we have

$$|e_{n+1}| \leq M|e_n|^2, \tag{34}$$

which is what we would expect if Newtons method converges quadratically. This result can be sued to give a mathematical proof of the convergence of Newtons method. Specically, we have the following theorem.

Theorem 3.6. *If f, f' and f'' are continuous in a neighborhood of a simple root r of f , then there is a $\delta > 0$ such that, if the initial guess x_0 satises $|r - x_0| \leq \delta$, then all subsequent approximations x_n satisfy the same inequality, and converge to r quadratically.*

In short, Newtons method always converges when the initial guess is 'sufficiently' close to the root.

The popularity of Newtons method is essentially based upon the fact that it converges quadratically. This is sometimes described by saying that the number of accurate digits in the answer doubles with each iteration. Quadratic convergence is more properly described as an asymptotic property, however, so that, in general, we cannot expect a doubling in the number of accurate digits on early iterations.

3.2.5 Choice of initial guess x_0.

When using Newtons method, it can be difficult to decide on a suitable initial guess. If x_0 is not close enough to the root, Newtons method will either diverge or converge to another root. It is sometimes helpful to have some insight into the shape of the graph of the function to guide the selection of an initial guess. Often the bisection method is used initially to obtain a suitable starting point, and Newtons method is then used to improve the precision.

4 The Secant Method

In comparison to Newton's method, the secant method uses the intersection of a secant line with the x-axis to update the approximation x_n. The corresponding iterative scheme is derived as follows. Assume that x_{n-1} and x_n are two approximations to the exact root r. We draw a secant line using the points $(x_{n-1}, f(x_{n-1}))$ and $(x_n, f(x_n))$ whose equation is given by

$$y - f(x_n) = m(x - x_n), \tag{35}$$

where

$$m = \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}} \tag{36}$$

is the slope of the straight line. The point of intersection of the line (35) with the x-axis, denoted by x_{n+1}, is given by

$$-f(x_n) = m(x_{n+1} - x_n),$$

or

$$x_{n+1} = x_n - \frac{f(x_n)}{m}.$$

Substituting for m from (36)

$$x_{n+1} = x_n - \frac{f(x_n)(x_n - x_{n-1})}{f(x_n) - f(x_{n-1})}.$$

Note that the secant method needs two initial points to start the iteration, while Newton's method needs only one. In addition, it can be proved that Newton's method converges more rapidly than the secant method. But the secant method does not involve the derivative of the function. In some applications when the derivative may not be available or is expensive to evaluate, the secant method is a viable alternative to Newton's method.

Exercise 4.1. Using the secant method, solve the floating sphere problem (3) in which the sphere's density is 1/3. Be sure to clearly indicate your choice of initial guess(es). Compare your results with those obtained using Newton's method and the bisection method. In addition to your results, please provide your code, in Matlab, clearly commented.

5 Reading Assignments/References:

1. About bisection method: follow the link `http://en.wikipedia.org/wiki/Bisection_method`.
2. About Newton's method: follow the link `http://en.wikipedia.org/wiki/Newton's_method`.
3. About secant method: follow the link `http://en.wikipedia.org/wiki/Secant_Method`.