Finding a Root for Nonlinear Equation

Numerical Methods

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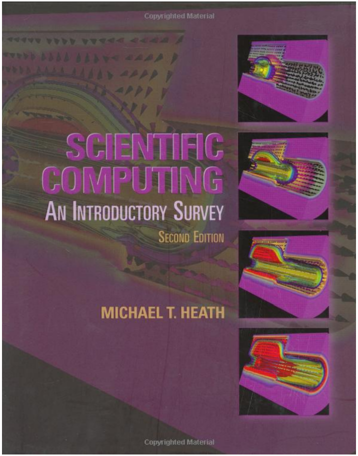
About

- This note discusses how to find a root of nonlinear equations using numerical methods.
- This note is based on Chapter 5. Nonlinear Equation of the following book.
- Heath, M. T. (2018). Scientific computing: an introductory survey, revised second edition. Society for Industrial and Applied Mathematics.



Theory

Definition: Root

- We are interested in finding values of x that solves an equation $f(x) = 0$ where $f(\cdot)$ is *nonlinear* function.
- Such a solution value x is called **solution** or **root** of the equation.

Number of solutions

- A number of solution for a nonlinear equation may vary.
- Example
  1. $x^2 - 4sin(x) = 0$ has a unique solution. ($x = 1.93375$)
  2. $e^x + 1 = 0$ has no solution.
  3. $x^2 - 4sin(x) = 0$ has two solutions.
  4. $x^3 + 6x^2 + 11x - 6 = 0$ has three solutions.
  5. $sin(x) = 0$ has infinitely many solutions.

Simple root and multiple root

- If $f(x^*) = 0$ and $f'(x^*) \neq 0$, then x^* is said to be a **simple root**.
- A solution that satisfies both equation $f(x^*) = 0$ and $f'(x^*) = 0$ called a **multiple root**.
- If $f(x^*) = f'(x^*) = 0$ but $f''(x^*) \neq 0$, then x^* is said to be a *multiplicity* 2.
- If $f(x^*) = f'(x^*) = f''(x^*) = 0$ but $f'''(x^*) \neq 0$, then x^* is said to be a *multiplicity* 3.

Multiple roots

1. The quadratic equation $x^2 - 2x + 1 = 0$ has a root of multiplicity two, $x = 1$.
2. The cubic equation $x^3 - 3x^2 + 3x - 1 = 0$ has a root of multiplicity three, $x = 1$.

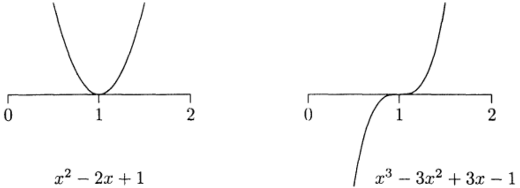


Figure 5.2: Two nonlinear functions, each having a multiple root.

- There is no *sign change* around the root of left figure. This limits applicable numerical methods.

Theorem: Intermediate Value Theorem

- If f is continuous on a closed interval $[a, b]$, and c lies between $f(a)$ and $f(b)$, then there is a value $x^* \in [a, b]$ s.t. $f(x^*) = c$.
- If $f(a)$ and $f(b)$ differ in sign, then by taking $c = 0$ in the theorem we can conclude that there must be a *root* within the interval $[a, b]$.
- Such an interval $[a, b]$ for which the sign of f differs contains a solution.

Definition: Contractive mapping

- A function $g : \mathbb{R} \rightarrow \mathbb{R}$ is **contractive** on a set $S \subseteq \mathbb{R}$, if there is a constant γ, with $0 < \gamma < 1$, such that $||g(x) - g(z)|| \leq \gamma ||x - z||$ for all $x, z \in S$.

Definition: Fixed point

- **A fixed point** of g is any value x such that $g(x) = x$.

Theorem: Contractive mapping theorem

- If g is contractive on a closed set $S \subseteq \mathbb{R}$ and $g(S) \subseteq S$, then g has a unique fixed point in S.
- Thus, if f has the form $f(x) = x - g(x)$, where g is contractive on a closed set $S \subseteq \mathbb{R}$, with $g(S) \subseteq S$, then $f(x) = 0$ has a unique solution in S, namely the fixed point of g.

A sketch of fixed-point iteration

- In order to find a root for $f(x) = 0$, fixed-point algorithm goes as follows.
  - *i)* Express the equation in a form of $f(x) = x - g(x)$
  - *ii)* (where $g(x)$ is contractive)
  - *iii)* Then, find the fixed point of g, i.e. $g(x) = x$.
  - *iv)* The fixed point of g solves $f(x) = 0$.

Goal

- Given a continuous, nonlinear, and univariate function $f : \mathbb{R} \to \mathbb{R}$, we seek a point $x^* \in \mathbb{R}$ s.t. $f(x^*) = 0$.
- This note presents the following four solution methods.
  1. Interval Bisection
  2. Fixed-Point Iteration
  3. Newton's Method
  4. Secant Method

1. Interval Bisection

Motivation

- We seek a *very short interval* $[a, b]$ in which f has a change of sign at both ends.
- Since the function is continuous, the intermediate value theorem guarantees the root is contained in the interval $[a, b]$.

Interval bisection *method*

i) begins with an initial interval that contains a root and

ii) successively halves the interval

iii) until the interval is short enough (i.e. $< tol$)

```
## 1. Interval Bisection
while (b-a > tol) do
  m=a+(b-a)/2 # m is midpoint of [a,b]
  if sgn(f(a))=sgn(f(m)) then
    a=m # so that [m,b] becomes new interval
  else
    b=m # so that [a,m] becomes new interval
  end
end
```

Example. $f(x) = x^2 - 4sin(x) = 0$

- With `a=1`, `b=3`, and `tol=0.01`

```
f <- function (x) { return(x^2 - 4*sin(x)) }; a = 1; b = 3; tol = 0.01
print(paste0("Initial interval: [", a, ",", b, "]"))
```

```
 "Initial interval: [1,3]"
```

```
while (b-a > tol) {
  m <- a+(b-a)/2
  if (f(a)*f(m)>0) {
    a <- m
  } else {
    b <- m
  }
  print(paste0("Current interval: [", a, ",", b, "]"))
}
```

```
 "Current interval: [1,2]"
 "Current interval: [1.5,2]"
 "Current interval: [1.75,2]"
 "Current interval: [1.875,2]"
 "Current interval: [1.875,1.9375]"
 "Current interval: [1.90625,1.9375]"
 "Current interval: [1.921875,1.9375]"
 "Current interval: [1.9296875,1.9375]"
```

Discussion

- The bisection method makes no use of function value except for the signs.
- This makes convergence rate low.
- With an initial interval $[a, b]$, length of interval after k-th iteration is $(b-a)/2^k$.

Exercise. Use the above method to find that $x = 0.567$ *approximately solves a nonlinear equation* $f(x) = e^{-x} - x = 0$.

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2. Fixed-Point Iteration

Motivation

- Remind that the interval bisection method does not make use of function value except for signs. This results in the lower convergence rate.
- The fixed-point iteration does make use of function values.

Development

- Remind that, for a function $g : \mathbb{R} \to \mathbb{R}$, a value x such that $x = g(x)$ is called a *fixed point* of the function g.
- For any given equation $f(x) = 0$, we can convert the problem into a form of $x = g(x)$, where the function g is *contractive* at the solution x^*.

Preparation of $x = g(x)$

- One needs to convert the original problem $f(x) = 0$ into the form of $x = g(x)$. This conversion process is not difficult.
- For example, by letting $g(x) := f(x) + x$, the original problem is converted to a fixed point problem of $x = g(x)$.
- The conversion is not unique, as will be discussed.

Fixed-Point Iteration *method*

i) Rearrange the equation $f(x) = 0$ in the form of $x = g(x)$.

ii) Choose the following.

- x_0: initial guess of solution
- tol: tolerable error
- N: maximum iterations

iii) Repeat the iteration scheme $x_{k+1} = g(x_k)$ until $|f(x)| \leq$ `tol` or `iter` $> N$

```
## 2. Fixed Point Iteration
while (f(x_old) > tol) or (iter <= N) do
  x_new <- g(x_old) # repeat the iteration scheme
  x_old <- x_new
  iter <- iter + 1
end
```

Example. $f(x) = x^2 - x - 2 = 0$

- The equation $x^2 - x - 2 = 0$ is converted to $x^2 = x + 2$, which is converted to $x = 1 + 2/x$.
- Thus, we let $g(x) = 1 + 2/x$
- With the setting of `x0=1`, `tol=0.01`, and `N=5`

```
f <- function (x) { return (x^2-x-2) }
g <- function (x) { return (1+2/x) }
x_old <- 1;
tol <- 0.01
N <- 5;
iter <- 0;
print(paste0("x_old:", x_old,
             " f(x_old):", f(x_old),
             " g(x_old):", g(x_old)))
```

```
"x_old:1 f(x_old):-2 g(x_old):3"
```

```
while ((abs(f(x_old)) > tol) || (iter <= N)) {
  x_new <- g(x_old) # repeat the iteration scheme
  x_old <- x_new
  iter <- iter + 1
  print(paste0("x_old:", round(x_old, 3),
               " f(x_old):", round(f(x_old), 3),
               " g(x_old):", round(g(x_old), 3)))
}
```

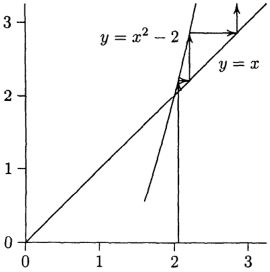
```
"x_old:3 f(x_old):4 g(x_old):1.667"
"x_old:1.667 f(x_old):-0.889 g(x_old):2.2"
"x_old:2.2 f(x_old):0.64 g(x_old):1.909"
"x_old:1.909 f(x_old):-0.264 g(x_old):2.048"
"x_old:2.048 f(x_old):0.145 g(x_old):1.977"
"x_old:1.977 f(x_old):-0.069 g(x_old):2.012"
"x_old:2.012 f(x_old):0.035 g(x_old):1.994"
"x_old:1.994 f(x_old):-0.018 g(x_old):2.003"
"x_old:2.003 f(x_old):0.009 g(x_old):1.999"
```

Convergence and divergence

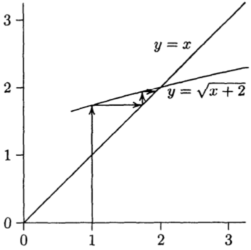
- If $x^* = g(x^*)$ and $|g'(x^*)| < 1$, then the iterative scheme is *locally convergent*, i.e., there is an interval containing x^* s.t. fixed-point iteration with g **converges** if started at a point within that interval.
- If $|g'(x^*)| > 1$, then fixed-point iteration with g **diverges**.

Four different approaches for $f(x) = x^2 - x - 2 = 0$

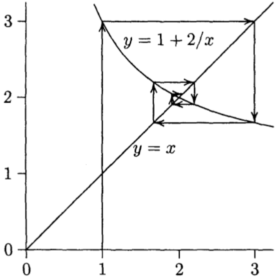
1. $x^2 - x - 2 = 0 \Longrightarrow x = x^2 - 2$
   $\Longrightarrow g_1(x) = x^2 - 2$
   - $g_1'(x) = 2x$, $g_1'(2) = 4$
   - It diverges because $|g_1'(2)| > 1$.



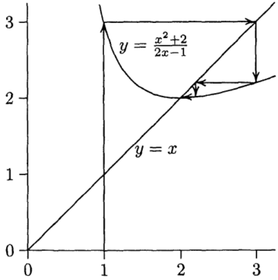
2. $x^2 = x + 2 \Longrightarrow x = \sqrt{x+2} \Longrightarrow$
   $g_2(x) = \sqrt{x+2}$
   - $g_2'(x) = \frac{1}{(2\sqrt{x+2})}$, $g_2'(2) = \frac{1}{4}$
   - It converges linearly.



3. $x^2 = x + 2 \Longrightarrow x = 1 + \frac{2}{x} \Longrightarrow$
   $g_3(x) = 1 + \frac{2}{x}$
- $g_3'(x) = \frac{-2}{x^2}$, $g_3'(2) = -\frac{1}{2}$
- It converges linearly.



4. $2x^2 - x^2 - x - 2 = 0 \Longrightarrow$
   $2x^2 - x = x^2 + 2 \Longrightarrow x = \frac{x^2+2}{2x-1}$
   $\Longrightarrow g_4(x) = \frac{x^2+2}{2x-1}$
- $g_4'(x) = \frac{2x^2-2x-4}{(2x-1)^2}$, $g_4'(2) = 0$
- It converges quadratically.



3. Newton's Method

Motivation

- Taylor's 1st order expansion goes as follows.

$$f(x+h) \approx f(x) + f'(x) \cdot h$$

- We can replace the *nonlinear function* f with *linear function* using its derivative.

Development

- We can view Newton's method as a systematic way of transforming a nonlinear equation $f(x) = 0$ into a fixed-point problem $x = g(x)$, where

$$g(x) = x - \frac{f(x)}{f'(x)}$$

- This method approximates the function f near x_k by the tangent line at $f(x_k)$.
- Then, the root of this tangent line becomes the next approximate solution.
- Repeat this process.

Newton's Method

i) Rearrange the equation $f(x) = 0$ in the form of $x = g(x)$, where $g(x) = x - \frac{f(x)}{f'(x)}$

ii) Choose the followings.

- $x_{\texttt{old}}$: initial guess of solution
- `tol`: tolerable error
- `N`: maximum iterations

iii) Repeat the iteration scheme $x_{k+1} = g(x_k)$ until $|f(x)| \leq$ `tol` or `iter` $> N$

```
## 3. Newton's Method
x_old <- initial guess
while (|f(x)| > tol) or (iter <= N)  do
  x_new <- x_old - f(x_old)/f'(x_old)
  iter <- iter+1
  x_old <- x_new
end
```

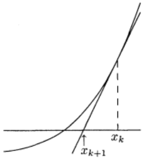


Figure 5.6: Newton's method for solving nonlinear equation.

Example. $f(x) = x^2 - 4sin(x) = 0$

- With x_old=3, tol=0.001

```
f <- function (x) { return(x^2 - 4*sin(x)) }
df <- function (x) { return(2*x - 4*cos(x))}
x_old <- 3; tol <- 0.001; N <- 3; iter <- 0;
print(paste0("x:", x_old, " f(x):", f(x_old)))
```

```
 "x:3 f(x):8.43551996776053"
```

```
while((abs(f(x_old))>tol) & (iter<=N)){
  x_new <- x_old - f(x_old)/df(x_old)
  x_old <- x_new
  iter <- iter + 1
  print(paste0("x:", x_new, " f(x):", f(x_new)))
}
```

```
 "x:2.15305769201339 f(x):1.29477250528657"
 "x:1.9540386420058 f(x):0.108438553394625"
 "x:1.93397153275207 f(x):0.00115163152386399"
 "x:1.93375378855763 f(x):0.000000136054946420217"
```

```
print(paste0("The root is ", x_new))
```

```
 "The root is 1.93375378855763"
```

Discussion

- The Newton's method has its drawback that both the function and its derivative must be evaluated at each iteration.
- Newton's method is fast, but requires its derivative analytically available.

Exercise. Use the above method to find that $x = 0.567$ *approximately solves a nonlinear equation* $f(x) = e^{-x} - x = 0$.

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4. Secant Method

Motivation

- A derivative of a function may be inconvenient or expensive to evaluate.
- So, secant method uses a better idea that is to use the finite difference approximation instead.

$$f'(x_k) \approx \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}$$

- The secant method can be interpreted as approximating the function f by the secant line through the previous two iterations.
- Then take the root of the resulting linear function to be the next approximate solution.

Secant Method

i) Choose the followings.

- $x_{\mathtt{old}}$: 0-th initial guess of solution
- $x_{\mathtt{new}}$: 1-st initial guess of solution
- `tol`: tolerable error
- `N`: maximum iterations

ii) Repeat the iteration scheme

$$x_{next} = x_{new} - f(x_{new}) \cdot \frac{x_{new} - x_{old}}{f(x_{new}) - f(x_{old})}$$

and update x_{old} and x_{new} until $|x_{new} - x_{old}| \leq$ `tol` or `iter` $> N$

```
## 4. Secant Method
x_old <- 0th initial guess
x_new <- 1st initial guess
while (|x_new-x_old)| > tol) or (iter <= N)  do
  x_next = x_new-f(x_new)*(x_new-x_old)/(f(x_new)-f(x_old))
  x_old = x_new
  x_new = x_next
end
```

Example. $f(x) = x^2 - 4sin(x) = 0$

- With x_old=1, x_new=3

```
f <- function (x) { return(x^2 - 4*sin(x)) }
x_old <- 1; x_new <- 3; tol <- 0.1; N <- 5; iter <- 0;
print(paste0(iter,"-th iter: ", "x_old:", x_old," x_new:", x_new, " f(x_old):", f(x_old)))
```

```
"0-th iter: x_old:1 x_new:3 f(x_old):-2.36588393923159"
```

```
while ((abs(x_new-x_old) > tol) & (iter <= N)) {
  x_next = x_new-f(x_new)*(x_new-x_old)/(f(x_new)-f(x_old))
  x_old = x_new
  x_new = x_next
  iter <- iter+1
  print(paste0(iter,"-th iter: ", "x_old:", x_old, " x_new:", x_new, " f(x_old):", f(x_old)))}
```

```
"1-th iter: x_old:3 x_new:1.43806971012353 f(x_old):8.43551996776053"
"2-th iter: x_old:1.43806971012353 x_new:1.72480462104936 f(x_old):-1.89677449157582"
"3-th iter: x_old:1.72480462104936 x_new:2.02983325288416 f(x_old):-0.977705597349626"
"4-th iter: x_old:2.02983325288416 x_new:1.92204417896096 f(x_old):0.534304487516024"
"5-th iter: x_old:1.92204417896096 x_new:1.93317401864344 f(x_old):-0.0615225574089555"
```

```
print(paste0("The root is ", x_new))
```

```
"The root is 1.93317401864344"
```

Discussion

- Compared with Newton's method, the secant method has
  - the advantage of requiring only one new function evaluation per iteration.
  - the disadvantages of requiring two starting guesses and converging somewhat more slowly.
- By using secant method, there is no need for the process of rearranging the function $f(x)$ to $g(x)$.

Exercise. Use the above method to find that $x = 0.567$ *approximately solves a nonlinear equation* $f(x) = e^{-x} - x = 0$.
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Acknowledgement

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