CS321-002

Introduction to Numerical Methods

Lecture 2

Locating Roots of Equations

Professor Jun Zhang

Department of Computer Science
University of Kentucky
Lexington, KY 40506-0046

September 7, 2000

Roots of a Function

Let $f(x)$ is a function that has values of opposite sign at the two ends of a given interval $[a, b]$ with $a < b$, i.e., $f(a) \cdot f(b) < 0$. If $f(x)$ is continuous on $[a, b]$, then there exits a number c in $[a, b]$ such that $f(c) = 0$

c is called a root of function $f(x) = 0$

example. the function

$$f(x) = x^2 + 2x - 3 = 0$$

has a root in the interval $[0, 2]$. It has two roots in the interval $[-5, 2]$

Remark: roots are not necessarily unique in a given interval

need some root finding algorithms for general functions

Bisection Method

Given an interval $[a, b]$ and a continuous function $f(x)$, if $f(a) \cdot f(b) < 0$, then $f(x)$ must has a root in $[a, b]$. How to find it?

We suppose $f(a) > 0$ and $f(b) < 0$

Step 1. compute the midpoint $c = \frac{b+a}{2}$, stop if $\frac{|b-a|}{2}$ is small, and take c as the root

Step 2. evaluate $f(c)$, if $f(c) = 0$, a root is found

Step 3. if $f(c) \neq 0$, then either $f(c) > 0$ or $f(c) < 0$

Step 4. if $f(c) < 0$, a root must be in $[a, c]$

Step 4. Let $b \leftarrow c, f(b) \leftarrow f(c)$, go to Step 1

Convergence Analysis

let r be a root of $f(x)$ in the interval $[a_0, b_0]$. let $c_0 = \frac{a+b}{2}$ be the midpoint, then

$$|r - c_0| \le \frac{b_0 - a_0}{2}.$$

if we use the bisection algorithm, we compute and have $a_0, b_0, c_0, a_1, b_1, c_1, \ldots$, then

$$|r - c_n| \le \frac{b_n - a_n}{2} \qquad (n \ge 0)$$

since the interval is halved at each step, we have

$$b_n - a_n = \frac{b_{n-1} - a_{n-1}}{2} = \cdots = \frac{b_0 - a_0}{2^n}$$

hence

$$|r - c_n| \le \frac{b_0 - a_0}{2^{n+1}}$$

which is the maximum error if we take c_n as an approximate to the root r

Linear Convergence

a sequence $\{x_n\}$ has linear convergence to a limit x if there exists a constant C in the interval $[0, 1)$ such that

$$|x_{n+1} - x| \leq C|x_n - x| \qquad (n \geq 1)$$

by recursion, we have

$$\begin{aligned} |x_{n+1} - x| &\leq C|x_n - x| \leq C^2|x_{n-1} - x| \\ &\leq \cdots \leq C^n|x_1 - x| \end{aligned}$$

or equivalently, a linear convergence satisfies

$$|x_{n+1} - x| \leq A\,C^n \qquad (0 \leq C < 1)$$

for some positive number A

the bisection algorithm has a linear convergence rate with $C = \frac{1}{2}$ and $A = b_0 - a_0$

Stopping Criterion

what is our goal? when to stop? how many iterations?

our goal is to find $r \in [a, b]$ such that $f(r) = 0$

with bisection algorithm, we generate a sequence such that

$$|r - c_n| < \epsilon$$

for some prescribed number $\epsilon > 0$

i.e., we find a point c_n inside the interval $[a, b]$ that is very close to the root r. we then use c_n as an approximate to r

it is not guaranteed, however, that $f(c_n)$ is *very close* to 0

How Many Iterations

if we want the approximate root c_n is close to the true root r, i.e., we want

$$|r - c_n| < \epsilon,$$

then the number of bisection steps n satisfies

$$\frac{b-a}{2^{n+1}} < \epsilon$$

or

$$n > \frac{\log(b-a) - \log(2\epsilon)}{\log 2}$$

example. find a root in $[16, 17]$ up to machine single precision

$a = (10\ 000.0)_2, b = (10\ 001.0)_2$ so r must have a binary form $r = (10\ 100.***\dots)_2$. We have a total of 24 bits, 5 is already fixed. The accuracy will be up to another 19 bits, which is between 2^{-19} and 2^{-20}. we choose $\epsilon = 10^{-20}$. Since $b - a = 1$, we need $2^{n+1} > 2^{20}$, yielding $n \geq 20$

Newton's Method

given a function $f(x)$ and a point x_0, if we know the derivative of $f(x)$ at x_0, we can construct a linear function that passes through $(x_0, f(x_0))$ with a slope $f'(x_0) \neq 0$ as

$$l(x) = f'(x_0)(x - x_0) + f(x_0)$$

since $l(x)$ is close to $f(x)$ at x_0, if x_0 is close to r, we can use the root of $l(x)$ as an approximate to r, the root of $f(x)$

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

x_1 may not close to r enough, we repeat the procedure to find

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}, \ldots$$

under certain conditions, $\{x_n\}$ converges to r

From Taylor Series

if $f(x_0) \neq 0$, but x_0 is close to r, we may assume that they differ by h, i.e., $x_0 + h = r$, or

$$f(x_0 + h) = f(r) = 0$$

using Taylor series expansions

$$f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \cdots = 0$$

ignoring the higher order terms, we have

$$f(x_0) + hf'(x_0) = 0$$

or

$$h = -\frac{f(x_0)}{f'(x_0)}$$

since h does not satisfy $f(x_0 + h) = 0$, we use

$$x_1 = x_0 + h = x_0 - \frac{f(x_0)}{f'(x_0)}$$

as an approximate to r, and repeat the process

Fast Convergence

find a root for the following function $f(x)$, starting at $x_0 = 4$

$$\begin{aligned} f(x) &= x^3 - 2x^2 + x - 3 \\ f'(x) &= 3x^2 - 4x + 1 \end{aligned}$$

n	x_n	$f(x_n)$
0	4.0	33.0
1	3.0	9.0
2	2.4375	2.04
3	2.21303 27224 731445	0.256
4	2.17555 49386 143684	6.46×10^{-3}
5	2.17456 01006 550714	4.48×10^{-6}
6	2.17455 94102 932841	1.97×10^{-12}

each iteration gains double digits of accuracy and $f(x_n)$ decreases quadratically to 0