Root finding continued

Eugeniy E. Mikhailov

The College of William & Mary



Lecture 07

▲ 同 ト ▲ 三 ト

Secant method



$$x_{i+2} = x_{i+1} - f(x_{i+1}) \frac{x_{i+1} - x_i}{f(x_{i+1}) - f(x_i)}$$

Need to provide two starting points x_1 and x_2 . Secant method converges with $m = (1 + \sqrt{5})/2 \approx 1.618$

Eugeniy Mikhailov (W&M)

Practical Computing

Newton-Raphson method



$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

Need to provide a starting points x_1 and the derivative of the function. Newton-Raphson method converges quadratically (m = 2), m = 3),

Eugeniy Mikhailov (W&M)

Practical Computing

Lecture 07 3 / 9

Mathematical definition

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

The initial intent is to calculate it at very small h.

▲ 同 ト ▲ 三 ト

Mathematical definition

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

The initial intent is to calculate it at very small *h*. Remember about roundoff errors (HW01).

Mathematical definition

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

The initial intent is to calculate it at very small *h*. Remember about roundoff errors (HW01). For computers with *h* small enough f(x + h) - f(x) = 0.

Mathematical definition

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

The initial intent is to calculate it at very small *h*. Remember about roundoff errors (HW01). For computers with *h* small enough f(x + h) - f(x) = 0. Let's be smarter. Recall Taylor series expansion

$$f(x+h) = f(x) + \frac{f'(x)}{1!}h + \frac{f''(x)}{2!}h^2 + \cdots$$

Mathematical definition

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

The initial intent is to calculate it at very small *h*. Remember about roundoff errors (HW01). For computers with *h* small enough f(x + h) - f(x) = 0. Let's be smarter. Recall Taylor series expansion

$$f(x+h) = f(x) + \frac{f'(x)}{1!}h + \frac{f''(x)}{2!}h^2 + \cdots$$

So we can see

$$f'_c(x) = \frac{f(x+h) - f(x)}{h} = f'(x) + \frac{f''(x)}{2}h + \cdots$$

Here computed approximation and algorithm error

Mathematical definition

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

The initial intent is to calculate it at very small *h*. Remember about roundoff errors (HW01). For computers with *h* small enough f(x + h) - f(x) = 0. Let's be smarter. Recall Taylor series expansion

$$f(x + h) = f(x) + \frac{f'(x)}{1!}h + \frac{f''(x)}{2!}h^2 + \cdots$$

So we can see

$$f'_c(x) = \frac{f(x+h) - f(x)}{h} = f'(x) + \frac{f''(x)}{2}h + \cdots$$

Here computed approximation and algorithm error There is a range of optimal *h* when both the round off and the algorithm errors are small \log_{100}

$$f_c'(x) = \frac{f(x+h) - f(x)}{h}$$

Algorithm error

$$\varepsilon_{fd} \approx rac{f''(x)}{2}h$$

Eugeniy Mikhailov (W&M)

$$f_c'(x) = \frac{f(x+h) - f(x)}{h}$$

Algorithm error

$$\varepsilon_{fd} \approx \frac{f''(x)}{2}h$$

This is quite bad since error is proportional to *h*.

< (P) > < (P) > (P

$$f'_c(x) = \frac{f(x+h) - f(x)}{h}$$

Algorithm error

$$\varepsilon_{fd} \approx rac{f''(x)}{2}h$$

This is quite bad since error is proportional to *h*.

Example

$$f(x) = a + bx^2$$

$$f'_c(x) = \frac{f(x+h) - f(x)}{h}$$

Algorithm error

$$\varepsilon_{fd} \approx rac{f''(x)}{2}h$$

This is quite bad since error is proportional to *h*.

Example

$$f(x) = a + bx^2$$

 $f_c'(x) = bxh+bh$

$$f'_c(x) = \frac{f(x+h) - f(x)}{h}$$

Algorithm error

$$\varepsilon_{fd} \approx rac{f''(x)}{2}h$$

This is quite bad since error is proportional to *h*.

Example

$$f(x) = a + bx^2$$

 $f_c'(x) = bxh+bh$

So for small x, the algorithm error dominate our approximation!

Derivative via Central difference

$$f_c'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

Derivative via Central difference

$$f_c'(x) = \frac{f(x+h) - f(x-h)}{2h}$$



Bonus problem for the homework 03 (5 points)

Plot the \log_{10} of the absolute error of $\sin(x)$ derivative at $x = \pi/4$ calculated with forward and central difference methods vs the \log_{10} the *h* value. See loglog help for ploting with logarithmic axes. The values of *h* should cover the range 10^{-16} , 10^{-15} , $10^{-14} \cdots 10^{-1}$, 1. At the low end error will be dominated by round offs and at the higher by the algorithm error.

The minimum of the absolute error indicates optimal values of *h*.

Ridders method - the variation of false position

Solve f(x) = 0 with linear approximation of the function $g(x) = f(x) \exp(hQ)$

- bracket the root between x_1 and x_2
- 2 evaluate function in the mid point $x_3 = (x_1 + x_2)/2$
- Ind new approximation for the root

$$x_4 = x_3 + sign(f_1 - f_2) \frac{f_3}{\sqrt{f_3^2 - f_1 f_2}} (x_3 - x_1)$$

where $f_1 = f(x_1), f_2 = f(x_2), f_3 = f(x_3)$

- Check if x₄ satisfies convergence condition
- re bracket the root using

•
$$x_4$$
 and $f_4 = f(x_4)$

• whichever of (*x*₁, *x*₂, *x*₃) is closer to *x*₄ and provides proper bracket.

proceed to step 1

Nice parts: x_4 is guaranteed to be inside the bracket, convergence of the algorithm is quadratic m = 2. But it requires evaluation of the f(x)twice for f_2 and f_4 thus actually $m = \sqrt{2}$.

Root finding algorithm gotchas

Eugeniy Mikhailov (W&M)

<ロト

Bracketing algorithm are bullet proof and will always converge, however false position algorithm could be slow.



Bracketing algorithm are bullet proof and will always converge, however false position algorithm could be slow.



Newton-Raphson and secant algorithm are usually fast but starting points need to be close enough to the root.



Root bracketing algorithms

- bisection
- false position
- Ridders

Pro

 robust i.e. always converge.

Contra

- usually slower convergence
- require initial bracketing

Non bracketing algorithms

- Newton-Raphson
- secant

Pro

- faster
- no need to bracket (just give a reasonable starting point)

< 同 ト < 三 ト

Contra

may not converge