

## Root finding continued

Eugeniy E. Mikhailov

The College of William & Mary



Lecture 06

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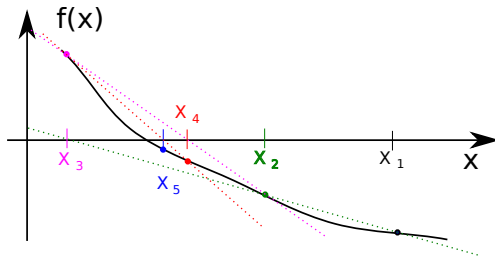
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### Secant method



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

Need to provide two starting points  $x_1$  and  $x_2$ .

Secant method converges with  $m = (1 + \sqrt{5})/2 \approx 1.618$

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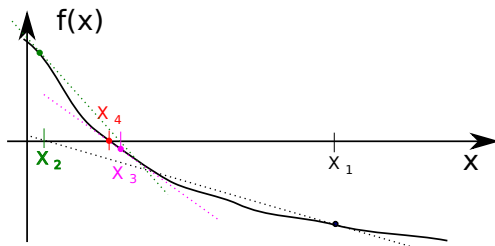
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### Newton-Raphson method



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

Need to provide a starting points  $x_1$  and the derivative of the function.

Newton-Raphson method converges quadratically ( $m = 2$ ).

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### Numerical derivative of a function

Mathematical definition

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

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

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Remember about roundoff errors (HW01).

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Let's be smarter. Recall Taylor series expansion

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

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So we can see

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

Here **computed approximation** and **algorithm error**.

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Here **computed approximation** and **algorithm error**. There is a range of optimal  $h$  when both the round off and the algorithm errors are small.

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## Derivative via Forward difference

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

Algorithm error for small  $h$

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

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

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Example

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

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### Example

$$\begin{aligned} f(x) &= a + bx^2 \\ f(x+h) &= a + b(x+h)^2 = a + bx^2 + 2bxh + bh^2 \end{aligned}$$

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

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### Example

$$\begin{aligned} f(x) &= a + bx^2 \\ f(x+h) &= a + b(x+h)^2 = a + bx^2 + 2bxh + bh^2 \\ f'_c(x) &= \frac{f(x+h) - f(x)}{h} = 2bx + bh \end{aligned}$$

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

## Derivative via Central difference

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

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## Derivative via Central difference

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

### Algorithm error

$$\varepsilon_{cd} \approx \frac{f'''(x)}{6} h^2$$

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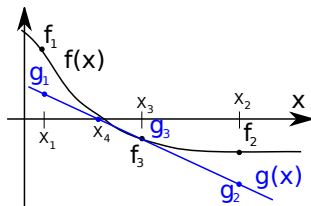
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## Ridders method - smart variation of false position

Solve  $f(x) = 0$  with the following approximation of the function  $f(x) = g(x) \exp(-C(x - x_r))$ , where  $g(x) = a + bx$  i.e. linear. In this case if  $g(x_0) = 0$  then  $f(x_0) = 0$ , but  $g(x) = 0$  is trivial to solve.



One can say that

$$g(x) = f(x) \exp(C(x - x_1)) = a + bx$$

We chose  $x_r = x_1$

## Ridders method implementation

- 1 bracket the root between  $x_1$  and  $x_2$ , i.e. function must have different signs at these points:  $f(x_1) \times f(x_2) < 0$
- 2 find the mid point  $x_3 = (x_1 + x_2)/2$
- 3 find new approximation for the root

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

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

- 4 check if  $x_4$  satisfies convergence condition and we should stop
- 5 rebracket the root, i.e. assign new  $x_1$  and  $x_2$ , using old values
  - one end of the bracket is  $x_4$  and  $f_4 = f(x_4)$
  - the other is whichever of  $(x_1, x_2, x_3)$  is closer to  $x_4$  and provides proper bracket.
- 6 proceed to step 2

Nice features:  $x_4$  is guaranteed to be inside the bracket, convergence of the algorithm is quadratic per cycle ( $m = 2$ ). But it requires evaluation of the  $f(x)$  twice for  $f_3$  and  $f_4$  thus it is actually  $m = \sqrt{2}$ .

## Root finding algorithm gotchas

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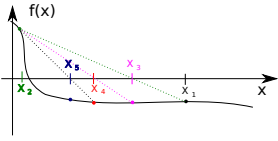
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## Root finding algorithm gotchas

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



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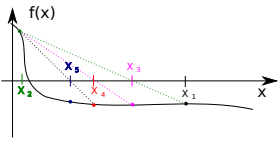
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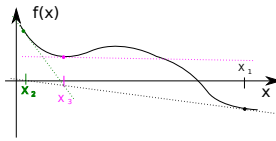
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## Root finding algorithm gotchas

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.



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## Root finding algorithms summary

### Root bracketing algorithms

- bisection
- false position
- Ridder's

### 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)

### Contra

- **may not converge**

See Matlab built in function `fzero` for equivalent tasks.

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