Root finding continued

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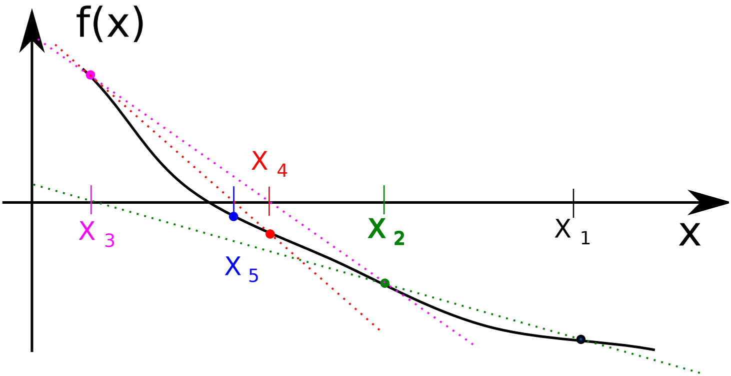
Lecture 06

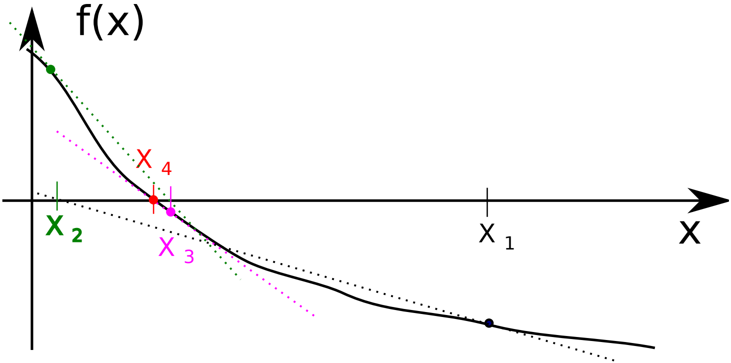
Secant method



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

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

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 ($m = 2$).

Numerical derivative of a function

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.

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Let's be smarter. Recall Taylor series expansion

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

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So we can see

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

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.

Derivative via Forward difference

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Algorithm error for small h

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

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

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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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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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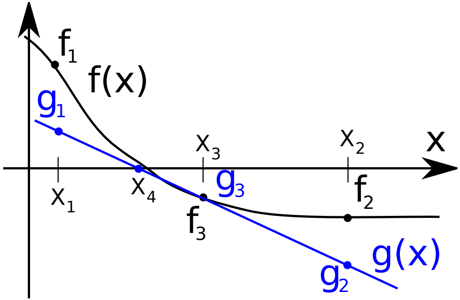
Algorithm error

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

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

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

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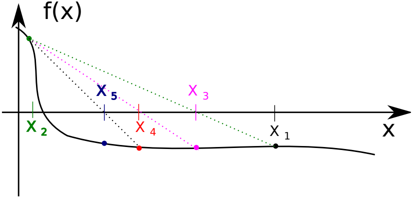
Bracketing algorithm are bullet proof and will always converge, however false position algorithm could be slow.



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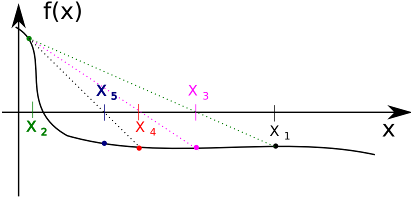
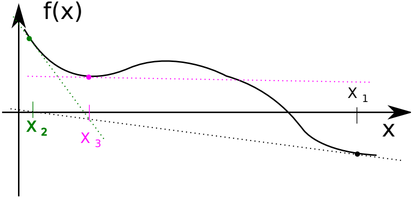


Newton-Raphson and secant algorithm are usually fast but starting points need to be close enough to the root.



Root finding algorithms summary

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)

Contra

- may not converge

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