Newton Method: Comments

$$x^{(i+1)} = x^{(i)} - \frac{f(x^{(i)})}{f'(x^{(i)})} \qquad \lim_{i\to\infty}\left|\frac{e^{(i+1)}}{\left[e^{(i)}\right]^2}\right| = \left|\frac{f''(\xi)}{2f'(\xi)}\right|$$

Writing as fixed-point scheme,

$$\phi(x) = x - \frac{f(x)}{f'(x)} \Rightarrow \phi'(x) = 1 - \frac{f'(x)}{f'(x)} + \frac{f(x)f''(x)}{\left[f'(x)\right]^2} \Rightarrow \phi'(\xi) = 0$$

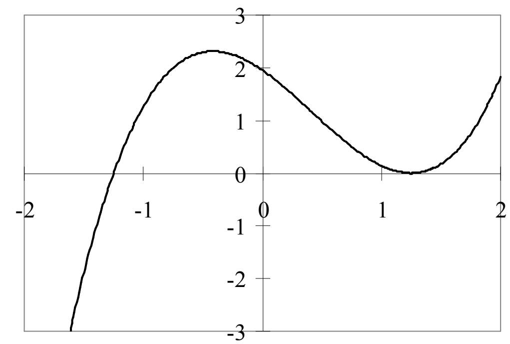
Second-order convergence.

- More computations, because of derivative
- May compute the derivative by taking a nearby point and doing a “finite” difference, but round-off errors
- Secant method has similar philosophy

Newton Method: Example

- Find the root near −1, starting with $x^{(0)}=-1$

$$f(x) = x^3 - 1.25020000x^2 - 1.56249999x + 1.95343750 = 0$$



$$\text{Iteration scheme} : x^{(i+1)} = x^{(i)} - \frac{f(x^{(i)})}{f'(x^{(i)})}$$

$$f'(x) = 3x^2 - 2.50040000x - 1.56249999$$

Iteration, i	$x^{(i)}$	f	f'	$x^{(i+1)}$	ε_a (%)
0	-1	1.265737	3.9379	-1.32142	24.32409
1	-1.32142	-0.47231	6.980078	-1.25376	5.397022
2	-1.25376	-0.02357	6.288132	-1.25001	0.299805
3	-1.25001	-7E-05	6.250613	-1.25	0.0009

- **To find root near 1:**
  (Note linear convergence, which is due to double root)

i	$x^{(i)}$	f	f'	$x^{(i+1)}$	ε_a (%)
0	1	0.140738	-1.0629	1.132409	11.69268
1	1.132409	0.032999	-0.54693	1.192745	5.058566
2	1.192745	0.008036	-0.27692	1.221763	2.375112
3	1.221763	0.001985	-0.13928	1.236013	1.152908
4	1.236013	0.000493	-0.06984	1.243076	0.56821

Newton Method: Multiple Roots

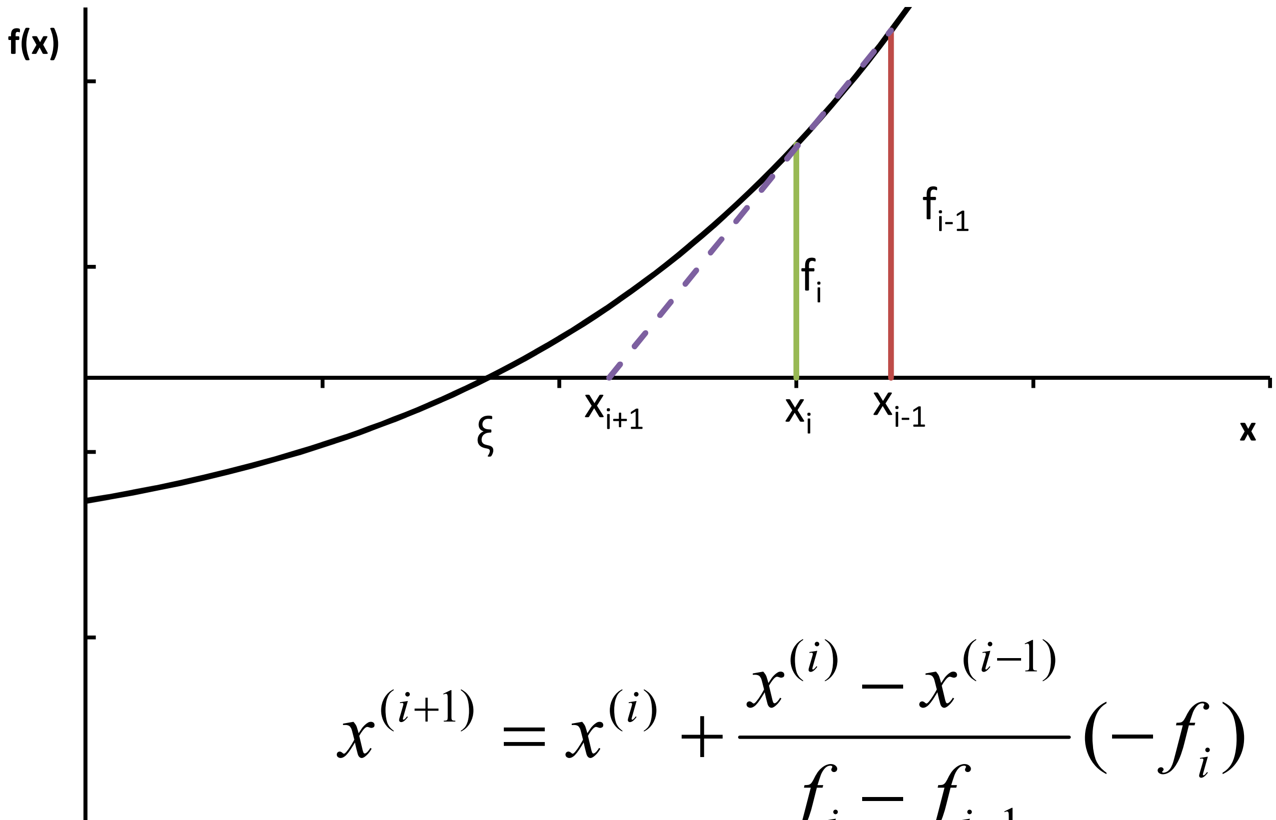
- Instead of f, find zeroes of f/f'

$$x^{(i+1)} = x^{(i)} - \frac{f(x^{(i)})/f'(x^{(i)})}{\frac{d}{dx}\left[f(x^{(i)})/f'(x^{(i)})\right]} = x^{(i)} - \frac{f_i f_i'}{(f_i')^2 - f_i f_i''}$$

$$f''(x) = 6x - 2.50040000$$

i	$x^{(i)}$	f	f'	f''	$x^{(i+1)}$	ε_a (%)
0	1.000000	0.140738	-1.062900	3.499600	1.234750	19.011928
1	1.234750	0.000585	-0.076048	4.908098	1.250052	1.224103
2	1.250052	0.000000	-0.000242	4.999910	1.250034	0.001403
3	1.250034	0.000000	-0.000329	4.999805	1.250029	0.000371

Secant Method: Algorithm

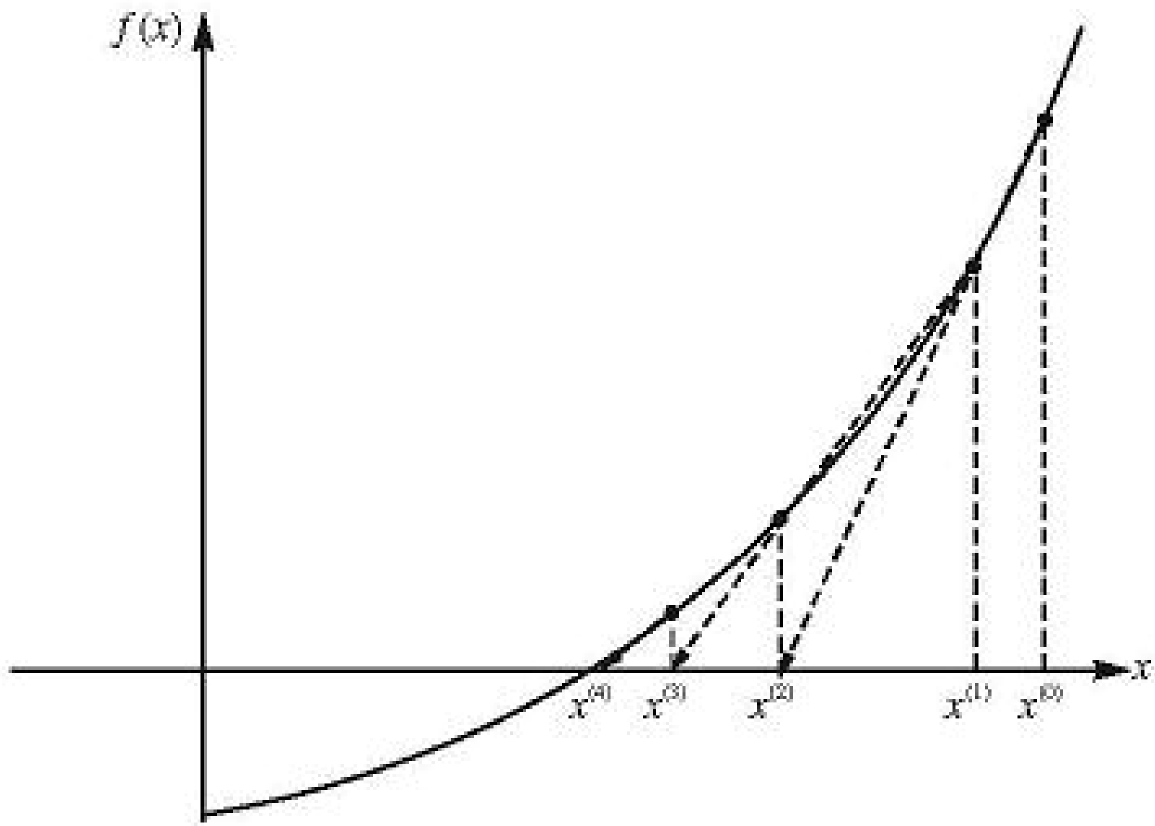


$$x^{(i+1)} = x^{(i)} + \frac{x^{(i)} - x^{(i-1)}}{f_i - f_{i-1}}(-f_i)$$

Difference from False Position method?

Not necessarily bracketing the root !

Secant Method: Iterations

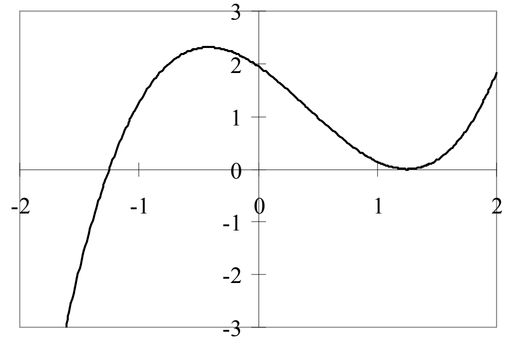


Generally, $x^{(i-1)}$ is discarded, when $x^{(i+1)}$ is computed. Sometimes, the point out of i-1, i, i+1, which has largest function magnitude is discarded.

Secant Method: Example

Find the root near −1, starting with $x^{(-1)}=-2$, $x^{(0)}=-1$

$$f(x) = x^3 - 1.25020000x^2 - 1.56249999x + 1.95343750 = 0$$



$$\text{Iteration scheme}: x^{(i+1)} = x^{(i)} + \frac{x^{(i)} - x^{(i-1)}}{f_i - f_{i-1}}(-f_i)$$

i	$x^{(i)}$	f	$x^{(i+1)}$	ε_a (%)
	-2	-7.92236		
0	-1	1.265737	-1.13776	12.10787
1	-1.13776	0.639987	-1.27865	11.01884
2	-1.27865	-0.18321	-1.24729	2.513998
3	-1.24729	0.016878	-1.24994	0.211612
4	-1.24994	0.000382	-1.25	0.004896

Secant Method: Error Analysis

- Similar to Linear interpolation, applied at the root, ξ,

$$0 = f_i + \left(\xi - x^{(i)}\right)\frac{f_i - f_{i-1}}{x^{(i)} - x^{(i-1)}} + \left(\xi - x^{(i)}\right)\left(\xi - x^{(i-1)}\right)\frac{f''(\zeta)}{2}; \zeta \in \left(x^{(i-1)}, x^{(i)}, \xi\right)$$

- Iteration $$x^{(i+1)} = x^{(i)} + \frac{x^{(i)} - x^{(i-1)}}{f_i - f_{i-1}}(-f_i)$$

- Error: $$\xi - x^{(i+1)} = \xi - x^{(i)} + f_i \frac{x^{(i)} - x^{(i-1)}}{f_i - f_{i-1}} \Rightarrow e^{(i+1)} = -e^{(i)} e^{(i-1)} \frac{f''(\zeta_1)}{2f'(\zeta_2)}$$

$$\zeta_1 \in \left(x^{(i-1)}, x^{(i)}, \xi\right); \zeta_2 \in \left(x^{(i-1)}, x^{(i)}\right)$$

- Recall: $$\lim_{i\to\infty}\frac{\left|e^{(i+1)}\right|}{\left|e^{(i)}\right|^p} = C; \Rightarrow \left|e^{(i+1)}\right| = C\left|e^{(i)}\right|^p \text{ and } \left|e^{(i-1)}\right| = \left|\frac{e^{(i)}}{C}\right|^{1/p}$$

Secant Method: Error Analysis

- As the iterations approach the root

$$C\left|e^{(i)}\right|^p = \left|e^{(i)}\right|\left|\frac{e^{(i)}}{C}\right|^{1/p}\left|\frac{f''(\xi)}{2f'(\xi)}\right| \Rightarrow C^{1+\frac{1}{p}}\left|e^{(i)}\right|^{p-1-\frac{1}{p}} = \left|\frac{f''(\xi)}{2f'(\xi)}\right|$$

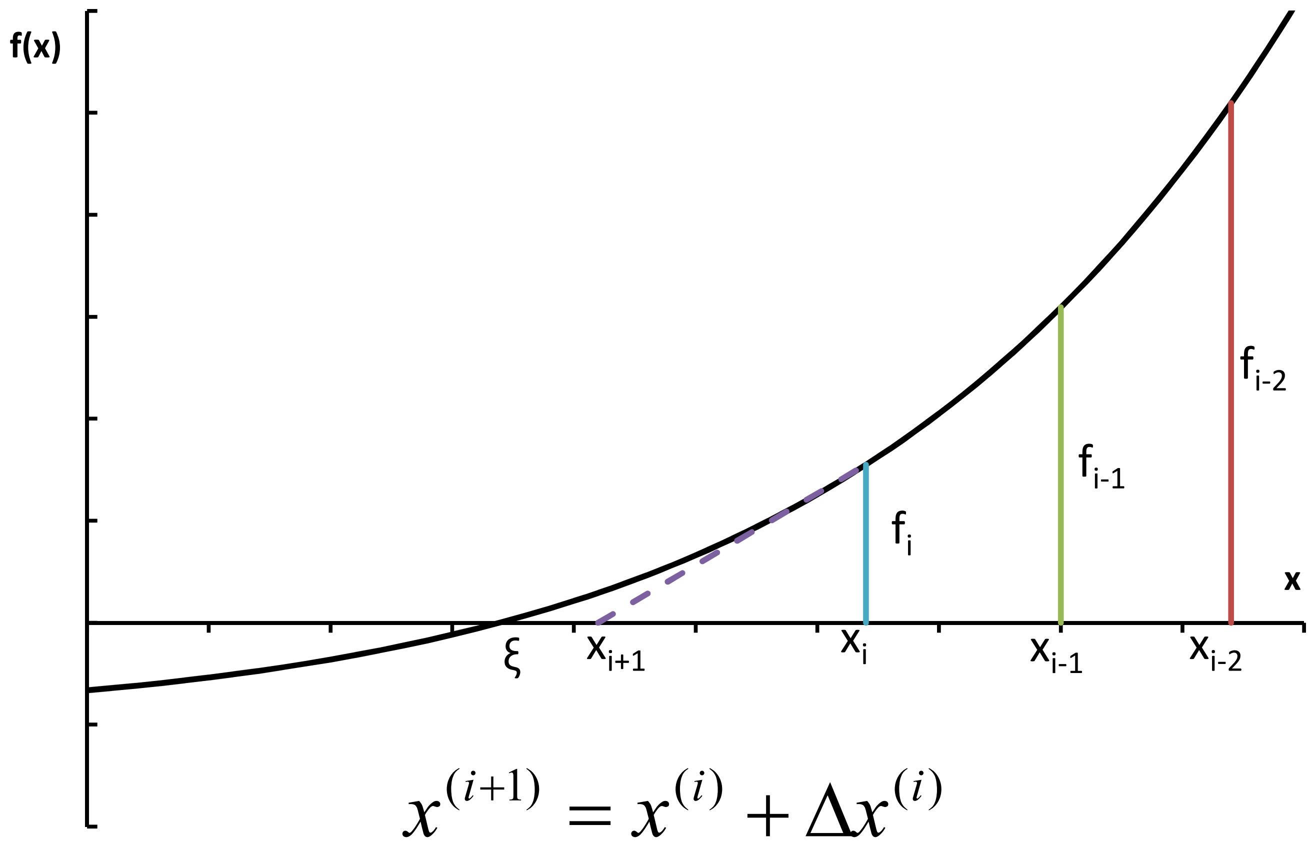
- Therefore, $p - 1 - 1/p = 0 \Rightarrow p=1.618$ (Golden Ratio)

and

$$C = \left|\frac{f''(\xi)}{2f'(\xi)}\right|^{0.618}$$

- Better than bisection and false position
- Not as good as Newton
- Can we improve the order by using three points and approximating the function by a quadratic instead of linear?

Muller Method: Algorithm



$$x^{(i+1)} = x^{(i)} + \Delta x^{(i)}$$

$\Delta x^{(i)}$ is obtained by interpolating a quadratic function through the three points (*i*, *i-1*, *i-2*) and finding its intersection with the *x*-axis

Muller Method: Algorithm

- It can be shown that

$$\Delta x^{(i)} = \frac{\pm\sqrt{b^2 - 4ac} - b}{2a} = -\frac{2c}{b \pm \sqrt{b^2 - 4ac}}$$

- Where

$$a = \frac{\dfrac{f_i - f_{i-1}}{x^{(i)} - x^{(i-1)}} - \dfrac{f_{i-1} - f_{i-2}}{x^{(i-1)} - x^{(i-2)}}}{x^{(i)} - x^{(i-2)}}$$

$$b = \frac{f_i - f_{i-1}}{x^{(i)} - x^{(i-1)}} + a\left(x^{(i)} - x^{(i-1)}\right)$$

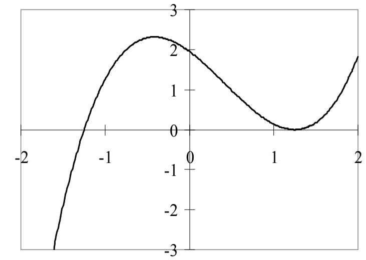
$$c = f_i$$

- Two roots, choose the smaller magnitude (i.e., +/- based on sign(b))

Muller Method: Example

Find the root near −1, starting with $x^{(-2)}=-2$, $x^{(-1)}=-1$, $x^{(0)}=0$

$$f(x) = x^3 - 1.25020000x^2 - 1.56249999x + 1.95343750 = 0$$



$$\text{Iteration scheme}: x^{(i+1)} = x^{(i)} - \frac{2c}{b \pm \sqrt{b^2 - 4ac}}$$

i	$x^{(i)}$	f	a	b	c	Δx	Δx2	$x^{(i+1)}$	ε_a (%)
	-2	-7.922							
	-1	1.2657							
0	0	1.9534	-4.25	-3.562	1.9534	0.3779	-1.216	0.3779	
1	0.3779	1.2383	-1.872	-2.6	1.2383	0.375	-1.764	0.753	49.808
2	0.753	0.495	-0.119	-2.027	0.495	0.2408	-17.23	0.9938	24.233
3	0.9938	0.1474	0.8745	-1.233	0.1474	0.1319	1.2778	1.1257	11.718
4	1.1257	0.0368	1.6223	-0.625	0.0368	0.0725	0.3126	1.1982	6.05
5	1.1982	0.0066	2.0675	-0.266	0.0066	0.0335	0.0953	1.2317	2.7176
6	1.2317	0.0008	2.3054	-0.095	0.0008	0.0131	0.028	1.2447	1.0488
7	1.2447	7E-05	2.4244	-0.027	7E-05	0.0042	0.0071	1.2489	0.3342

Muller Method: Error Analysis

- Quadratic interpolation, applied at the root, ξ,

$$0 = f_i + \left(\xi - x^{(i)}\right)\frac{f_i - f_{i-1}}{x^{(i)} - x^{(i-1)}} + \left(\xi - x^{(i)}\right)\left(\xi - x^{(i-1)}\right)\frac{\dfrac{f_i - f_{i-1}}{x^{(i)} - x^{(i-1)}} - \dfrac{f_{i-1} - f_{i-2}}{x^{(i-1)} - x^{(i-2)}}}{x^{(i)} - x^{(i-2)}}$$

$$+ \left(\xi - x^{(i)}\right)\left(\xi - x^{(i-1)}\right)\left(\xi - x^{(i-2)}\right)\frac{f'''(\zeta)}{6}; \zeta \in \left(x^{(i-2)}, x^{(i-1)}, x^{(i)}, \xi\right)$$

- From the Iteration scheme, it can be shown (as before) that

$$e^{(i+1)} = -e^{(i)}e^{(i-1)}e^{(i-2)}\,\frac{f'''(\xi)}{6f'(\xi)}$$

- Order of convergence: $p^3 - p^2 - p - 1=0 \Rightarrow p=1.839$

and

$$C = \left|\frac{f'''(\xi)}{6f'(\xi)}\right|^{0.4196}$$

- Better than Secant

Roots of polynomials: General

- Polynomial equations are very common in Eigenvalue problems and approximations of functions
- Any of the methods discussed so far should work
- After finding one root, we may ***deflate*** the polynomial and find other roots successively
- If some roots are complex, we may run into problems. This may happen even with polynomials which have all real coefficients.
- We will look at polynomials with real coefficients only
- The complex roots will occur in conjugate pairs, implying that a quadratic factor with real coefficients will be present

$$(x-[a+ib])(x-[a-ib]) = x^2 - 2ax + a^2 + b^2$$

- Bairstow Method

Roots of polynomials: Bairstow Method

- Find a quadratic factor of the polynomial *f(x) as* $x^2 - \alpha_1 x - \alpha_0$
- Find the two roots (real or complex conjugates) as

$$r_{1,2} = 0.5\left(\alpha_1 \pm \sqrt{\alpha_1^2 + 4\alpha_0}\right)$$

- Algorithm: Express the given function as $f(x) = \sum_{j=0}^{n} c_j x^j$

- Perform a synthetic division by the quadratic factor

$$x^2 - \alpha_1 x - \alpha_0 \overline{\big) c_n x^n + c_{n-1} x^{n-1} + c_{n-2} x^{n-2} + c_{n-3} x^{n-3} + \ldots + c_1 x + c_0} \Big(c_n x^{n-2} + \left(c_{n\text{-}1} + \alpha_1 c_n\right) x^{n-3} + ..$$

$$c_n x^n - \alpha_1 c_n x^{n-1} - \alpha_0 c_n x^{n-2}$$

$$\overline{\left(c_{n\text{-}1} + \alpha_1 c_n\right) x^{n-1} + \left(c_{n\text{-}2} + \alpha_0 c_n\right) x^{n-2} + c_{n-3} x^{n-3}}$$

$$\underline{\left(c_{n\text{-}1} + \alpha_1 c_n\right) x^{n-1} + \alpha_1 \left(c_{n\text{-}1} + \alpha_1 c_n\right) x^{n-2} + \alpha_0 \left(c_{n\text{-}1} + \alpha_1 c_n\right) x^{n-3}}$$