Nonlinear Equations

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Reactor Physics, KTH

Overview

- Scalar/Vector NLE
- Multiplicity
- Bracket
- Sensitivity/conditioning
- Bracketing vs. Open domain Methods
- Bisection, Secant, Newton's, Muller's
- Fixed Point Iterations, FPI
- Practical Considerations

Nonlinear Equations

$$f(x) = b \qquad\qquad f(x) \in C^1\left[c, d\right]$$

$$\mathbf{f}\left(\mathbf{x}\right) = \mathbf{b} \qquad \longleftrightarrow \qquad \begin{cases} f_1(x_1, \ldots, x_n) = b_1 \\ \vdots \\ f_n(x_1, \ldots, x_n) = b_n \end{cases}$$

Polynomial Equations

$$p_n(x) = a_n x^n + \ldots + a_1 x + a_0 = 0 \qquad a_n \neq 0$$

$$p_1(x) = a_1 x + a_0 = 0 \longrightarrow x = -a_0 / a_1$$

$$p_2(x) = a_2 x^2 + a_1 x + a_0 = 0 \longrightarrow x_{1,2} = \frac{-a_1 \pm \sqrt{a_1^2 - 4a_2 a_0}}{2a_2}$$

Cubic Equation

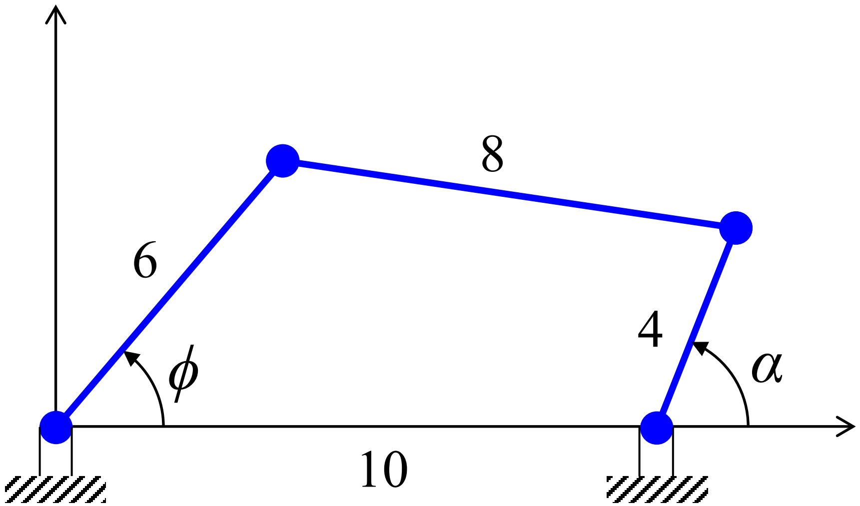
$$p_3(x) = ax^3 + bx^2 + cx + d = 0$$

$$x = t - \frac{b}{3a} \longrightarrow t^3 + pt + q = 0$$

$$p = \frac{3ac - b^2}{3a^2} \qquad q = \frac{2b^3 - 9abc + 27a^2 d}{27a^3}$$

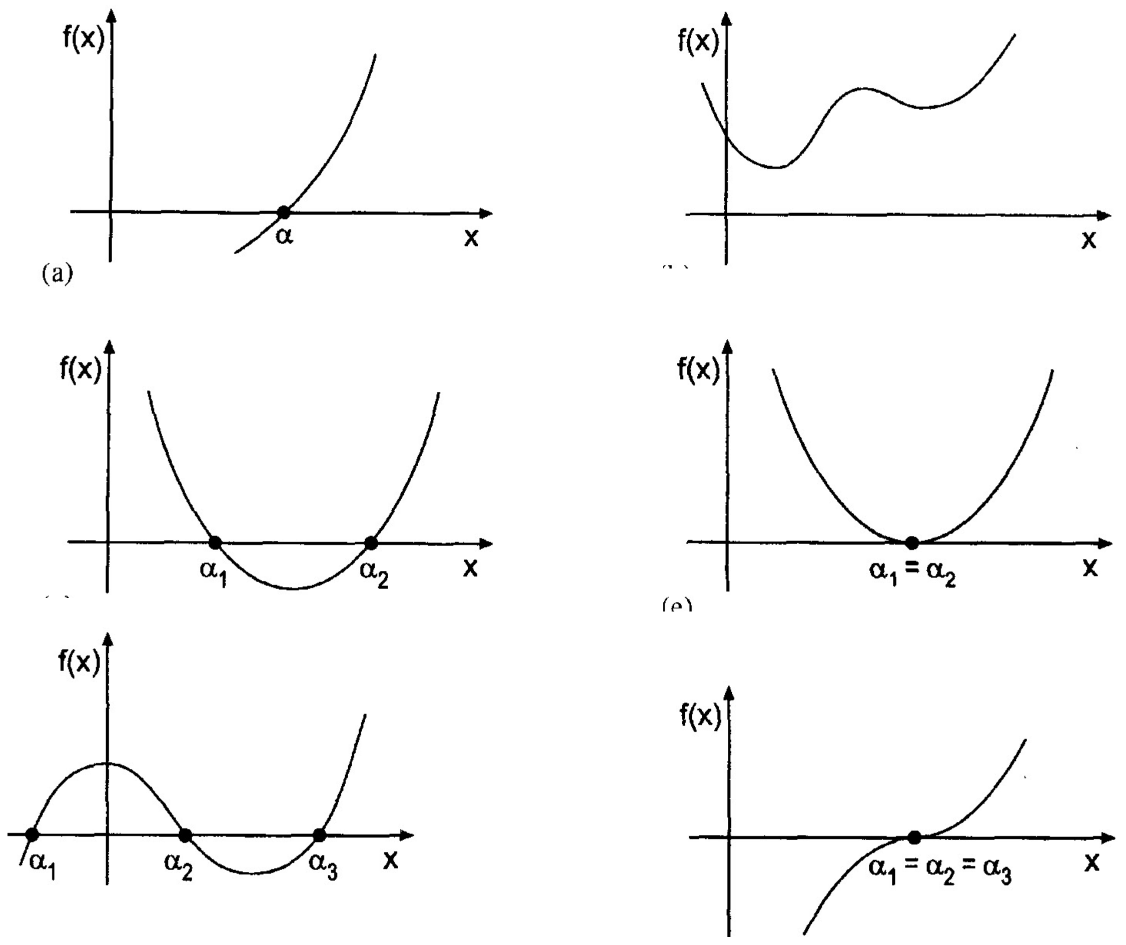
$$t = u + v \qquad u^3 = -\frac{q}{2} + \sqrt{\frac{q^2}{4} + \frac{p^3}{27}} \qquad v^3 = -\frac{q}{2} - \sqrt{\frac{q^2}{4} + \frac{p^3}{27}}$$

Four-Bar Linkage



$$10\cos\alpha - 15\cos\phi + 11 - 6\cos\left(\alpha - \phi\right) = 0$$

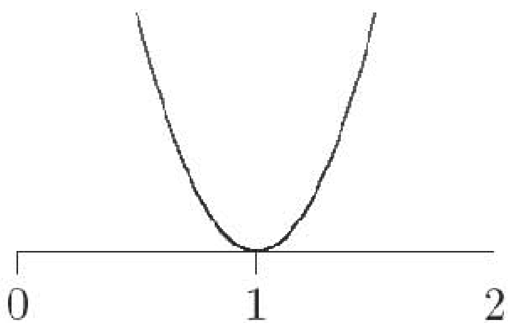
Types of Solutions



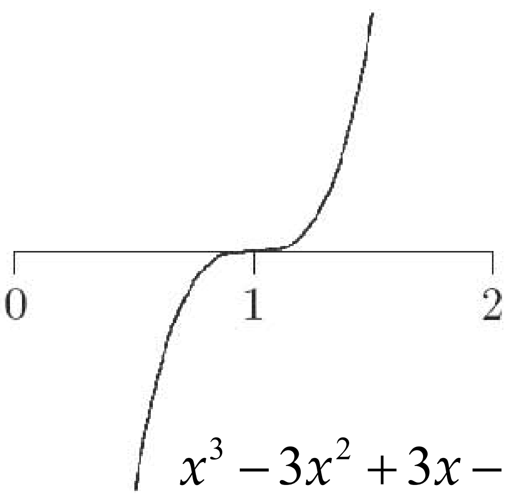
Multiplicity

$$f(\alpha) = f'(\alpha) = \ldots = f^{(m-1)}(\alpha) = 0 \qquad f^{(m)}(\alpha) \neq 0$$

$$f(\alpha) = 0 \qquad f'(\alpha) \neq 0 \longrightarrow m = 1$$



$$x^2 - 2x + 1 = 0$$



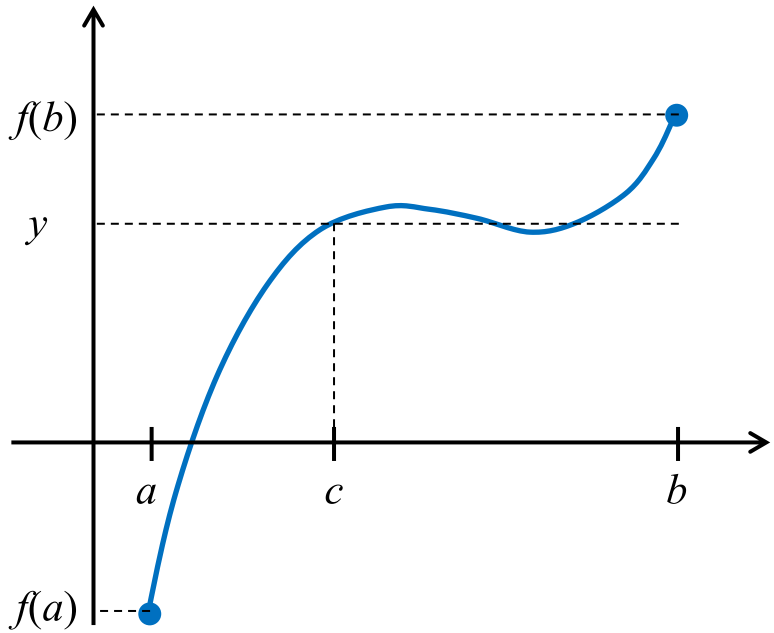
$$x^3 - 3x^2 + 3x - 1 = 0$$

Intermediate Value Theorem

Continuous function

$$\lim_{x \to c} f(x) = f(c)$$

Let $f(x)$ be a continuos function on $[a,b]$ then f realises every value between $f(a)$ and $f(b)$. More precisely, if y is a number between a and b, then there exists a number c, $a \le c \le b$, such that $y = f(c)$.



Sign Function

$$\operatorname{sgn}(x) = \operatorname{sign}(x) \equiv \begin{cases} -1 & x < 0 \\ 0 & x = 0 \\ +1 & x > 0 \end{cases}$$

Intermediate Value Theorem

If $f(x)$ is continuous and $\text{sign}[f(a)] \neq \text{sign}[f(b)]$ then there exists $a < x^* < b$ such that $f(x^*) = 0$.

An interval $[a,b]$ is said to be a bracket for $f(x)$ if $\text{sign}[f(a)] \neq \text{sign}[f(b)]$.

There is no simple analogue for n dimensions.

Sensitivity

$$f(x) = b$$

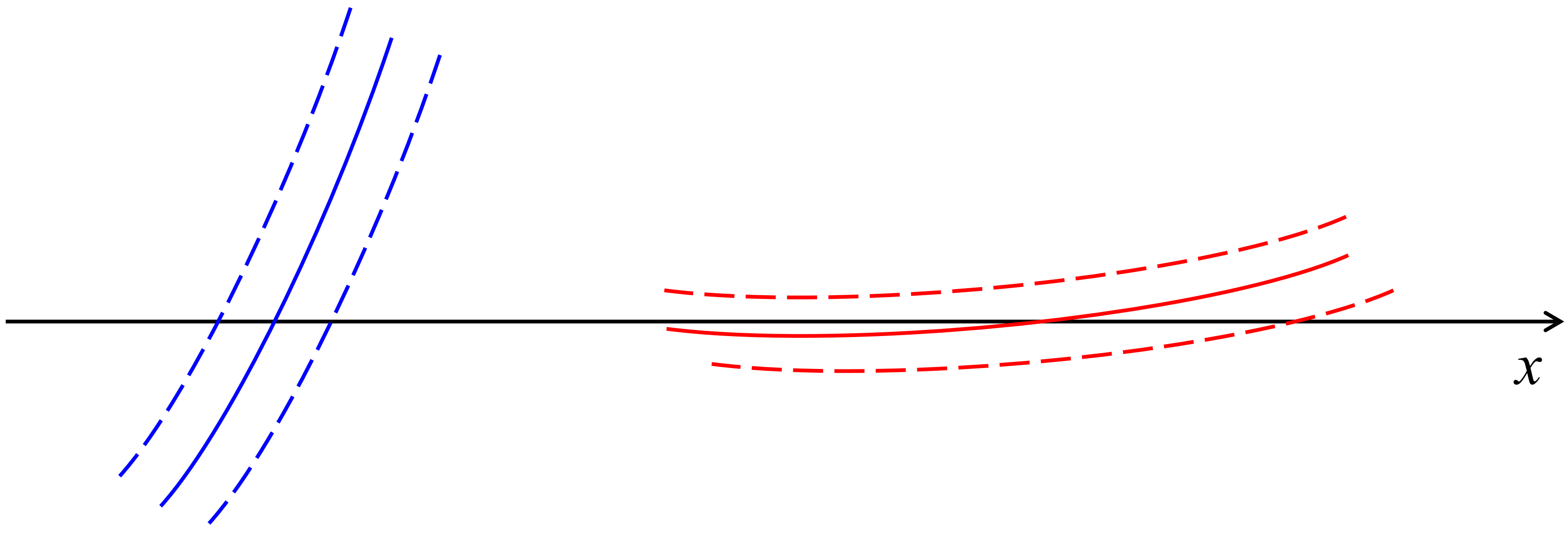
$$f(x+\delta x) = b + \delta b = f(x) + f'(x)\delta x + O\left(\delta x^2\right)$$

$$\delta b \approx f'(x)\delta x \longrightarrow \left|\delta x\right| \approx \frac{\left|\delta b\right|}{\left|f'(x)\right|} \longrightarrow \kappa_{abs}(x) \equiv \sup_{\delta \mathbf{b}} \frac{\left|\delta x\right|}{\left|\delta b\right|} \simeq \frac{1}{\left|f'(x)\right|}$$

$$\kappa_{abs}(\mathbf{x}) \equiv \sup_{\delta \mathbf{b}} \frac{\left\|\delta \mathbf{x}\right\|}{\left\|\delta \mathbf{b}\right\|} \simeq \left\|\mathbf{J}_{\mathbf{f}}^{-1}(\mathbf{x})\right\|; \qquad \kappa(\mathbf{x}) \equiv \sup_{\delta \mathbf{b}} \frac{\left\|\delta \mathbf{x}\right\| / \left\|\mathbf{x}\right\|}{\left\|\delta \mathbf{b}\right\| / \left\|\mathbf{b}\right\|} \cong \left\|\mathbf{J}_{\mathbf{f}}^{-1}(\mathbf{x})\right\| \frac{\left\|\mathbf{b}\right\|}{\left\|\mathbf{x}\right\|};$$

Conditioning

$$y = f(x) - b$$



Multiple Roots

$$b = f(x)$$

$$b + \delta b = f(x + \delta x) = f(x) + \frac{f^{(m)}(x)}{m!}(\delta x)^m + O\left((\delta x)^{m+1}\right)$$

$$\delta b \approx \frac{f^{(m)}(x)}{m!}(\delta x)^m \longrightarrow \delta x \approx \frac{(\delta b)^{1/m}}{\left[f^{(m)}(x)/m!\right]^{1/m}}$$

$$\kappa_{abs}(x) \equiv \frac{1}{\left[f^{(m)}(x)/m!\right]^{1/m}}$$

Iteration Sequence

$$\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(k)} \xrightarrow[k\to\infty]{} \mathbf{x}$$

$$\mathbf{e}^{(k)} = \mathbf{x}^{(k)} - \mathbf{x} \xrightarrow[k\to\infty]{} \mathbf{0}$$

1) Bounding the solution
   - Graphing
   - Incremental search
   - Past experience
   - Simplified model
   - Previous solution

2) Refining the solution
   - Closed domain (bracketing)
   - Open domain

Iteration Methods

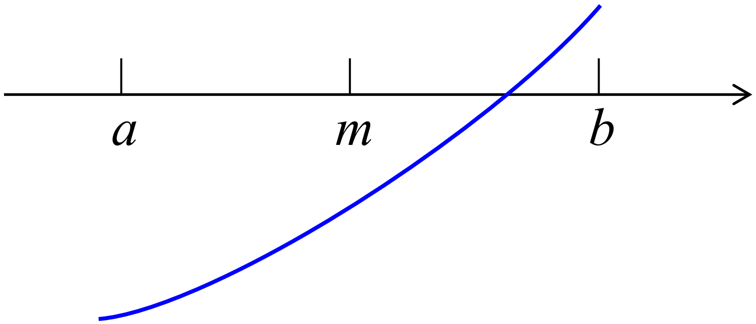
1) Closed domain (bracketing)
   - Interval halving (bisection)
   - False position (Regula falsi)
2) Open domain
   - Fixed point
   - Newton's method
   - Secant method
   - Brent's method

Rate of Convergence

$$\lim_{k\to\infty} \frac{\left\| \mathbf{e}^{(k+1)} \right\|}{\left\| \mathbf{e}^{(k)} \right\|^{p}} = C \neq 0$$

		Digits gained per iteration
• $p = 1$	Linear (C < 1)	Constant
• $p > 1$	Superlinear	Increasing
• $p = 2$	Quadratic	Doubles
• $p = 3$	Cubic	Triples

Bisection Method



Given a and b: $f(a)\cdot f(b) < 0$

```
while b - a > tol
   m = a + (b - a)/2;
   if sign(f(a)) == sign(f(m))
      a = m;
   else
      b = m;
   end
end
```

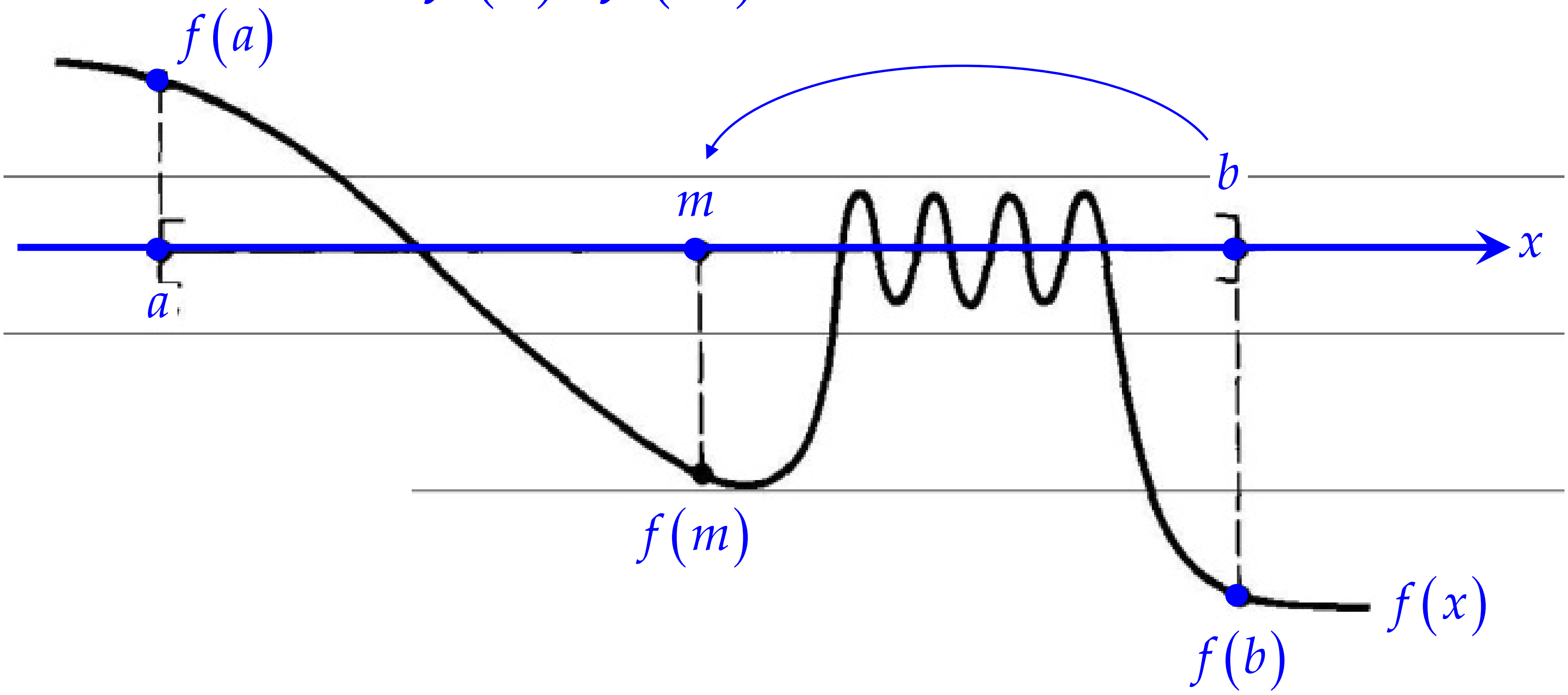
Convergence of BM

- BM makes no use of function, only signs
- BM is certain to converge but not very fast
- Interval is halved, $p = 1$, $C = 0.5$
- One bit of accuracy is gained
- After k iterations, $(b - a)/2^k$, irrespective f

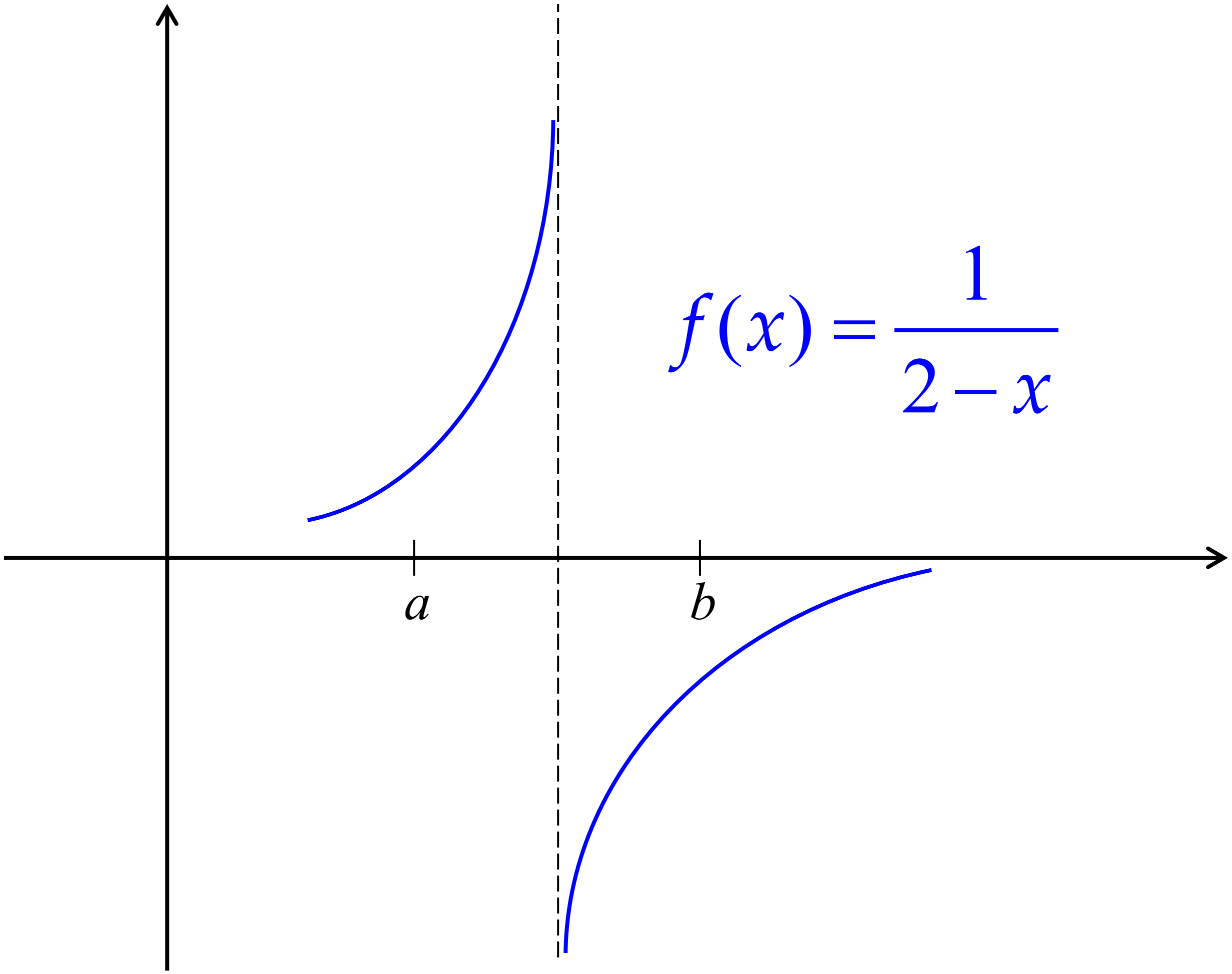
$$\frac{b-a}{2^k} < \varepsilon \longrightarrow k = \left\lceil \log_2 \frac{b-a}{\varepsilon} \right\rceil$$

Many Roots

$$f(a)\cdot f(m)<0 \longrightarrow b=m$$



Singularity



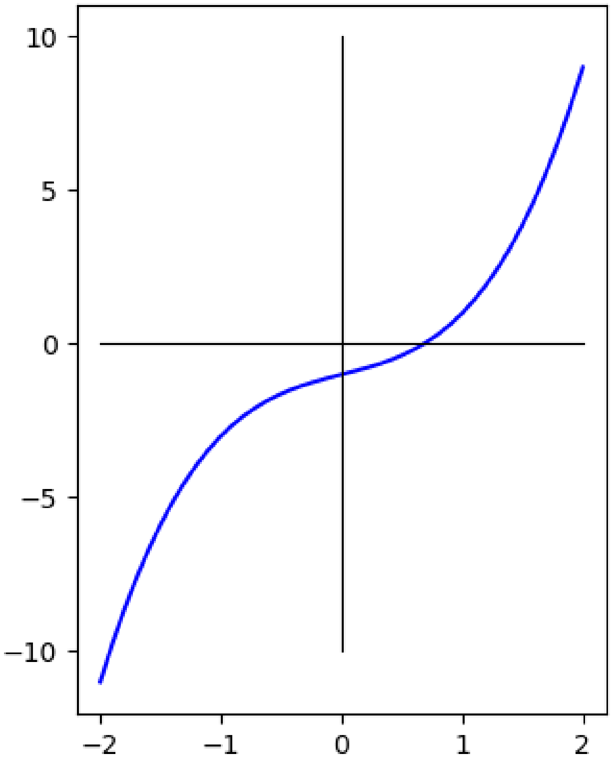
Termination

$$b - a < tol_x$$

$$f(m) < tol_y$$

Cubic Equation

$$f(x) = x^3 + x - 1 = 0 \qquad [0,1] \qquad f(0) = -1; \qquad f(1) = +1.$$



Scipione del Ferro (1465 – 1526)

Nicolo Tartaglia (1499/1500 – 1557)

Gerolamo Cardano, 1501 – 1576; cubic - 1545

$$x^3 + mx = n$$

$$x = \sqrt[3]{\frac{n}{2} + \sqrt{\left(\frac{n}{2}\right)^2 + \left(\frac{m}{3}\right)^3}} - \sqrt[3]{-\frac{n}{2} + \sqrt{\left(\frac{n}{2}\right)^2 + \left(\frac{m}{3}\right)^3}}$$

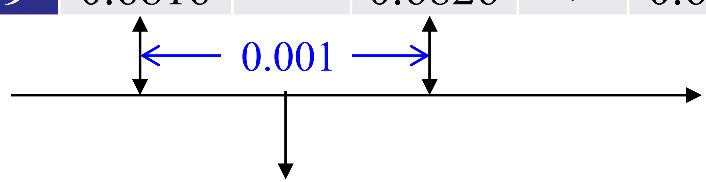
$$x = 0.6823278038280194$$

Example

$$f(x) = x^3 + x - 1 = 0 \qquad [0,1]$$

$$f(0) = -1; \qquad f(1) = +1.$$

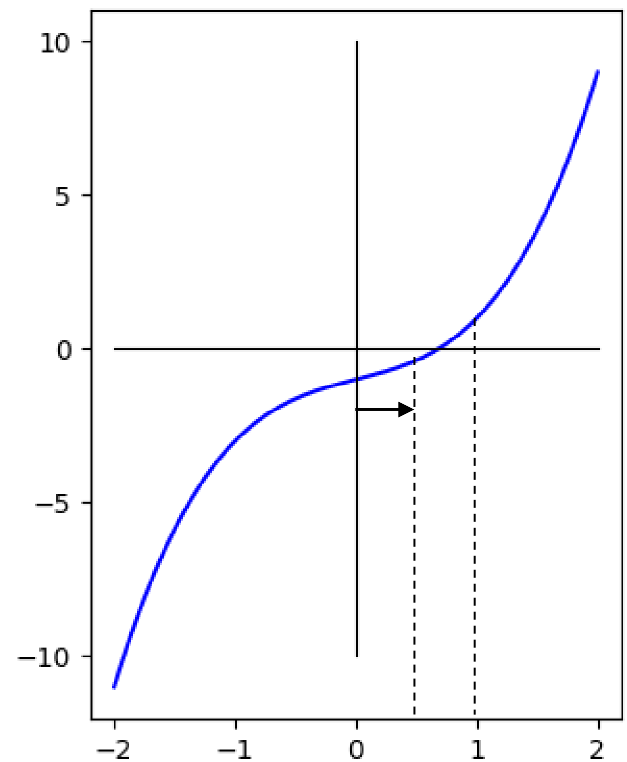
k	a_k	$f(a_k)$	c_k	$f(c_k)$	b_k	$f(a_k)$
0	0.0000	–	0.5000	–	1.0000	+
1	0.5000	–	0.7500	+	1.0000	+
2	0.5000	–	0.6250	–	0.7500	+
3	0.6250	–	0.6875	+	0.7500	+
4	0.6250	–	0.6562	–	0.6875	+
5	0.6562	–	0.6719	–	0.6875	+
6	0.6719	–	0.6797	–	0.6875	+
7	0.6797	–	0.6836	+	0.6875	+
8	0.6797	–	0.6816	–	0.6836	+
9	0.6816	–	0.6826	+	0.6836	+



$$x_c = 0.6821$$

$$x = 0.6821 \pm 0.0005$$

$$x = 0.6823278038280194$$



Efficiency

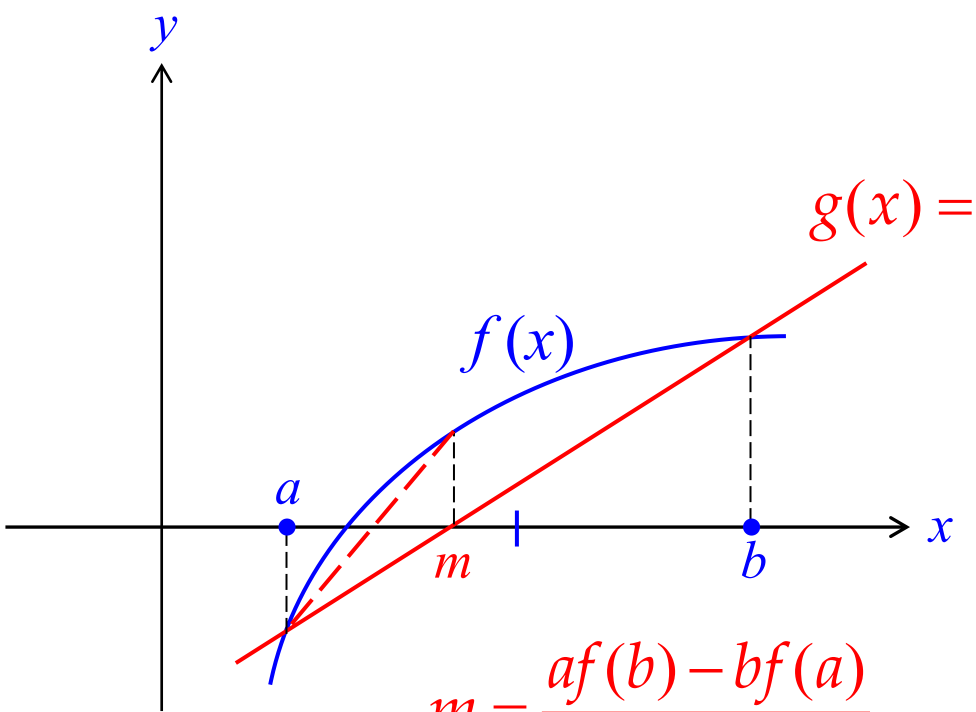
Solution error $$|x - x_c| < \frac{b-a}{2^{k+1}}$$

One function evaluation at each step cutting the uncertainty by 2.

A solution is **correct within** p **decimal places** if the error is less than 0.5×10^{-p}.

$$x = 0.6821 \pm 0.0005 = 0.6821 \pm 0.5 \times 10^{-3}$$

Improving Bisection Method



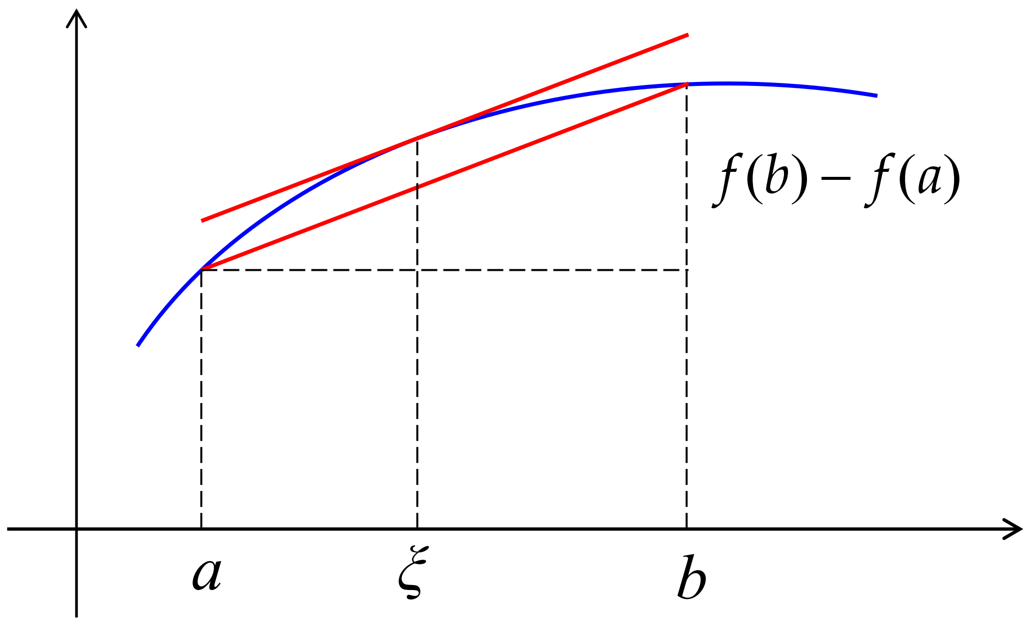
$$g(x) = \frac{f(b) - f(a)}{b - a} x + \frac{bf(a) - af(b)}{b - a}$$

$$m = \frac{af(b) - bf(a)}{f(b) - f(a)}$$

Mean Value Theorem

$$f(b)-f(a)=f'(\xi)\left(b-a\right)$$

$$\frac{f(b)-f(a)}{b-a}=f'(\xi)$$



Iterative Scheme

$$f(\alpha)=0 \longrightarrow f(\alpha)-f(x)=f'(\xi)\left(\alpha-x\right)$$

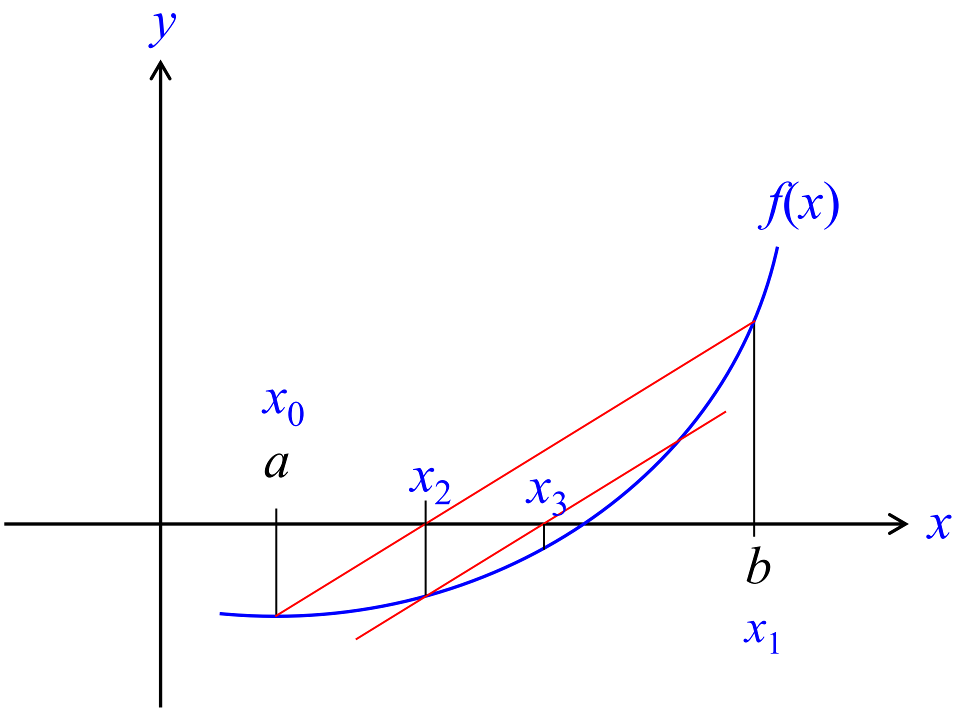
$$\alpha = x - \frac{f(x)}{f'(\xi)}$$

$$\tilde{\alpha} = x - \frac{f(x)}{q} \longrightarrow x_{k+1} = x_k - \frac{f(x_k)}{q_k}$$

Chord Method

$$x_{k+1} = x_k - \frac{f(x_k)}{q_k}$$

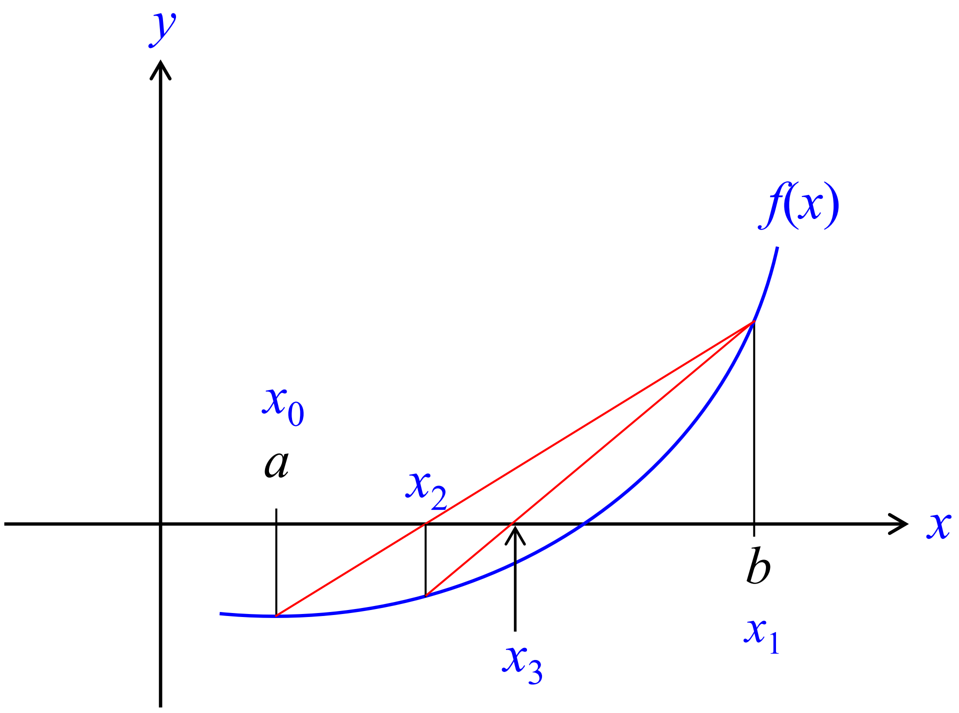
$$q_k = \frac{f(b) - f(a)}{b - a}$$



Secant Method

$$x_{k+1} = x_k - \frac{f(x_k)}{q_k}$$

$$q_k = \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}$$



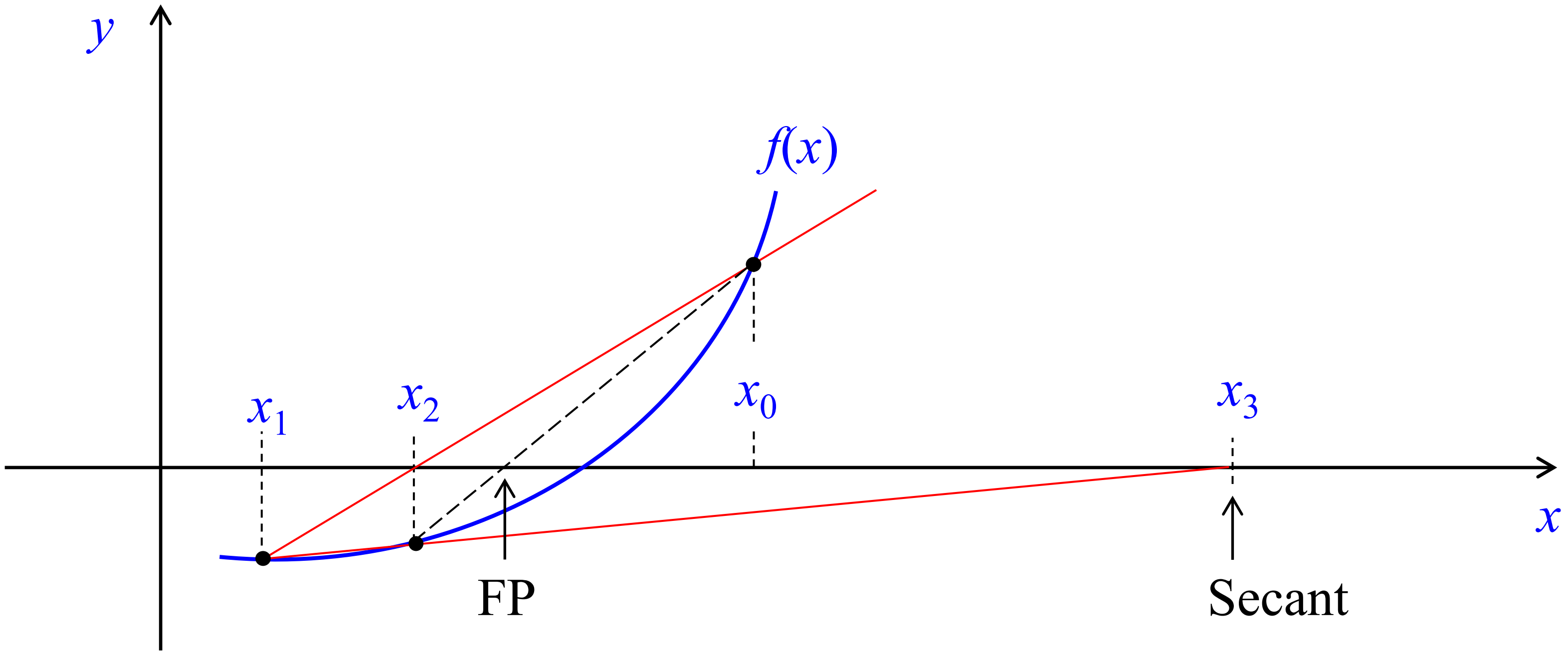
Algorithm

Given a and b: $f(a) \cdot f(b) < 0$

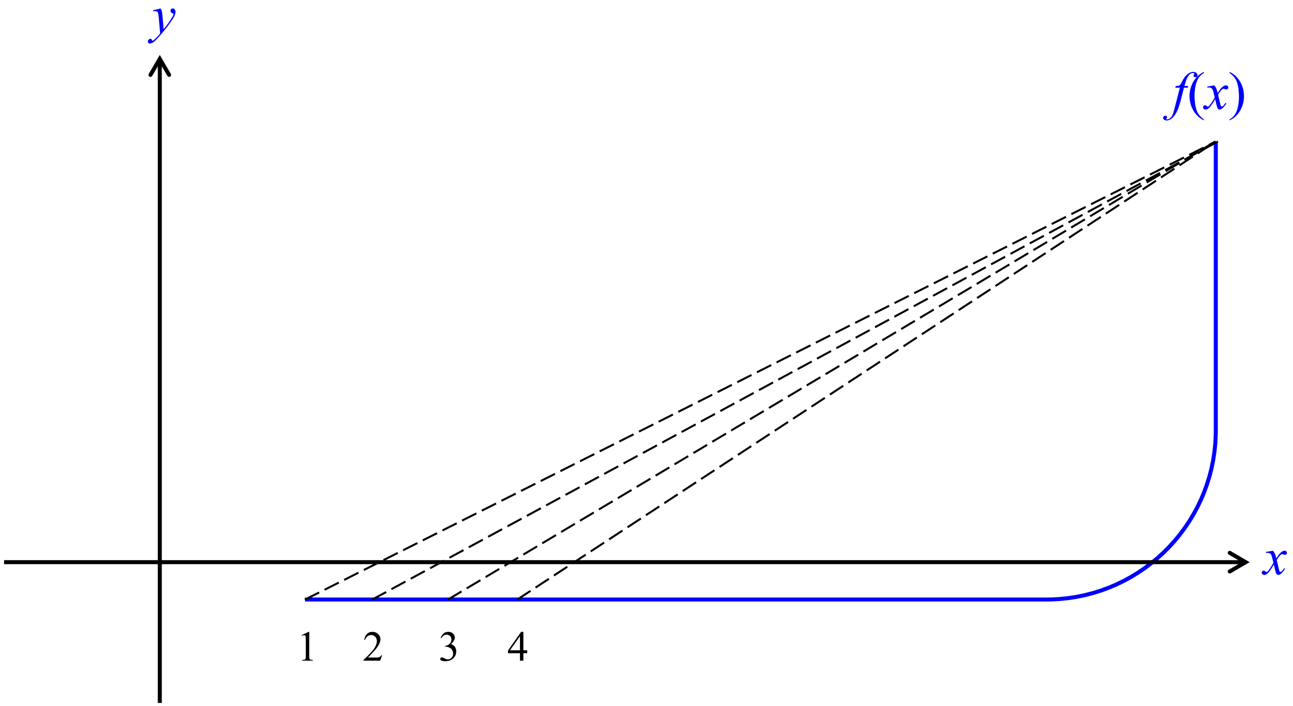
```
while b - a > tol
   ~~m = a + (b - a)/2;~~
   if sign(f(a)) == sign(f(m))
      a = m;
   else
      b = m;
   end
end
```

$$m = \frac{af(b) - bf(a)}{f(b) - f(a)}$$

False Position vs. Secant

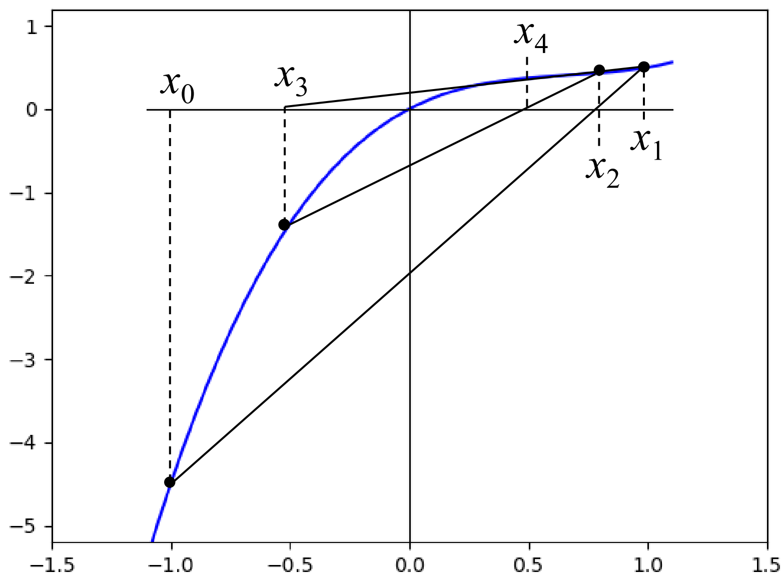


FP: Slow Convergence

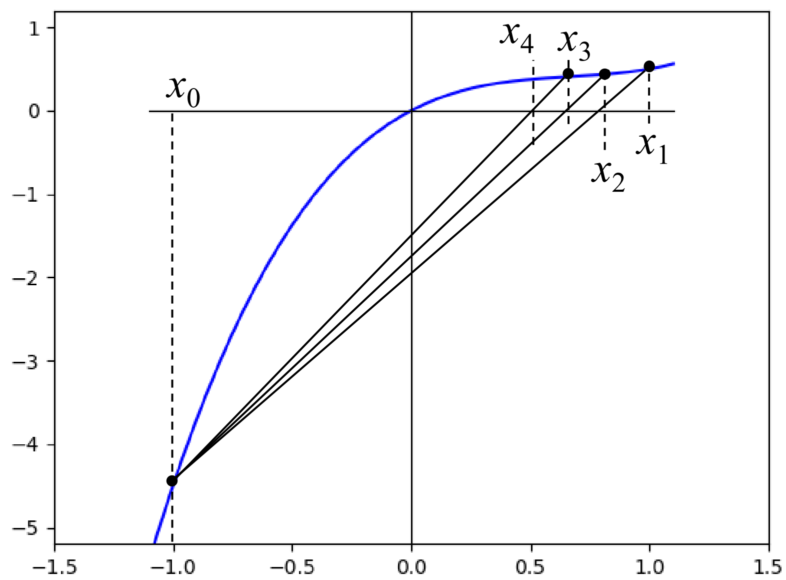


More Realistic Example

$$f(x) = x^3 - 2x^2 + \frac{3}{2}x = 0$$



Secant



False Position

Convergence Theorem for SM

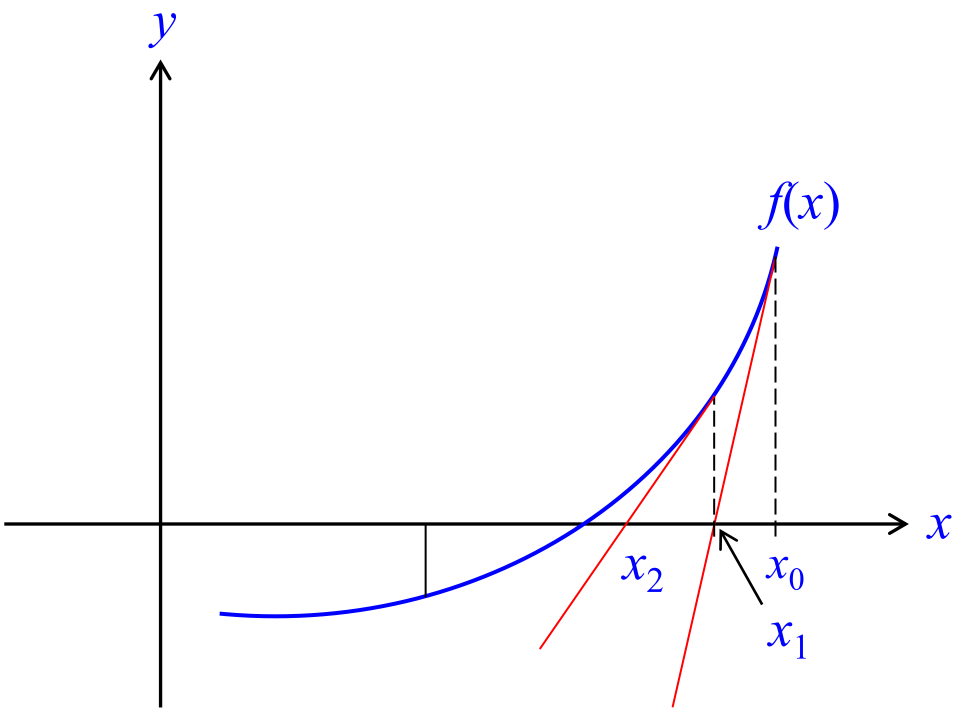
Secant method may produce iterates outside $[a,b]$ whereas BM and FPM always generates approximations inside $[a,b]$. BM and FPM are regarded as globally convergent.

Theorem. Let $f(x)$ be twice differentiable and $f''(\alpha) \neq 0$. Then if a and b are chosen sufficiently close to root then the secant methods converges to the solution with the order $p = \left(1+\sqrt{5}\right)/2 \simeq 1.63$

Newton's Method

$$x_{k+1} = x_k - \frac{f(x_k)}{q_k}$$

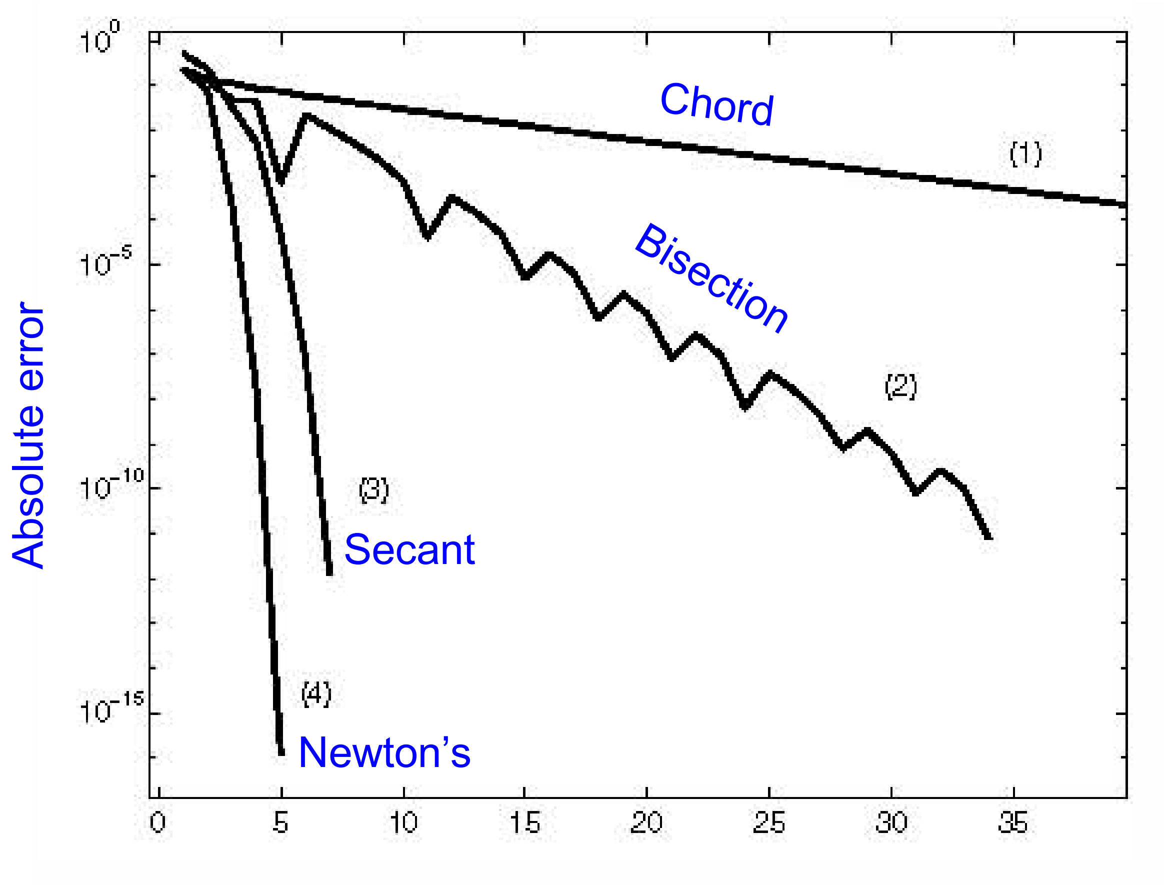
$$q_k = f'(x_k)$$



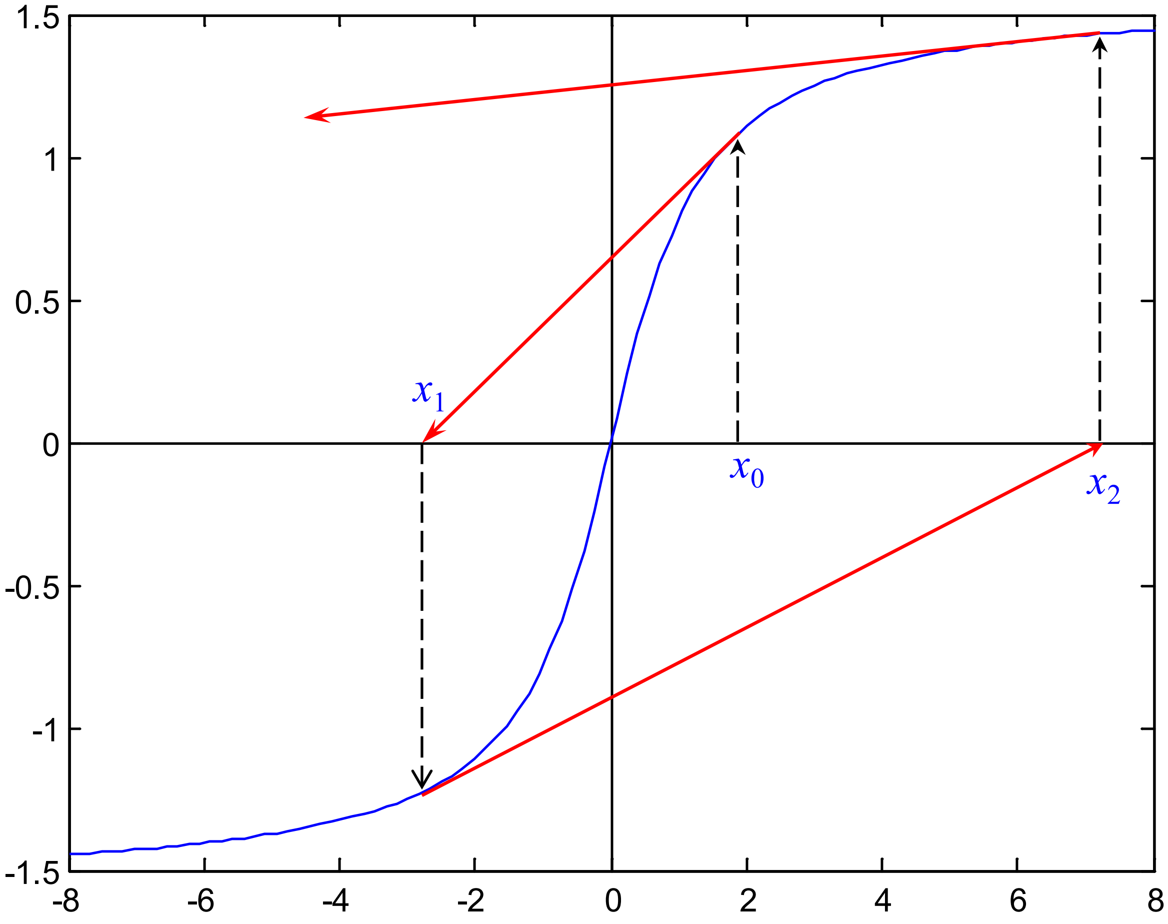
1) Open domain
2) Convergence order, $p = 2$

Numerical Example

$$f(x) = \cos^2(2x) - x^2 = 0 \qquad x \in [0, 3/2]$$



Divergence of Newton's



Multiple Roots in Newton's

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

Simple Multiple

$p = 2$ $p = 1$ $C = 1 - 1/m$

$$x_{k+1} = x_k - m\frac{f(x_k)}{f'(x_k)}$$

Simple Multiple

$p = 2$ $p = 2$

Modifications of Newton's

$$f(x) = (x-\alpha)^m h(x) \longrightarrow u(x) \equiv \frac{f(x)}{f'(x)} = \frac{(x-\alpha)h(x)}{mh(x) + (x-\alpha)h'(x)}$$

$$x_{k+1} = x_k - \frac{u(x_k)}{u'(x_k)}$$

$$x_{k+1} = x_k - m\frac{f(x_k)}{f'(x_k)}$$

$$x_{k+1} = x_k - \frac{f(x_k)f'(x_k)}{\left[f'(x_k)\right]^2 - f(x_k)f''(x_k)}$$

Error Analysis

$$0 = f(\alpha) = f(x_k) + f'(x_k)(\alpha - x_k) + \frac{1}{2!} f''(\xi_k)(\alpha - x_k)^2$$

$$\underbrace{x_k - \frac{f(x_k)}{f'(x_k)}}_{x_{k+1}} - \alpha = \frac{1}{2!} \frac{f''(\xi_k)}{f'(x_k)} (x_k - \alpha)^2$$

$$e_{k+1} = \frac{1}{2!} \frac{f''(\xi_k)}{f'(x_k)} [e_k]^2 \approx \frac{1}{2!} \frac{f''(x_k)}{f'(x_k)} [e_k]^2$$

Convergence Theorem

There exists an interval, $I = [\alpha - r, \alpha + r]$ such that

$$f'(x) \neq 0 \qquad \forall x \in I$$

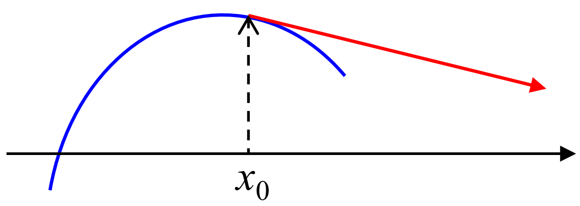
$$\left| f''(x) \right| \leq C \quad \forall x \in I$$

x_0 is sufficiently close to α.

Failure Analysis

Bad starting point

1) Not close enough
2) Iteration point is stationary, $f(x) = 1 - x^2$
3) Iteration enters a cycle

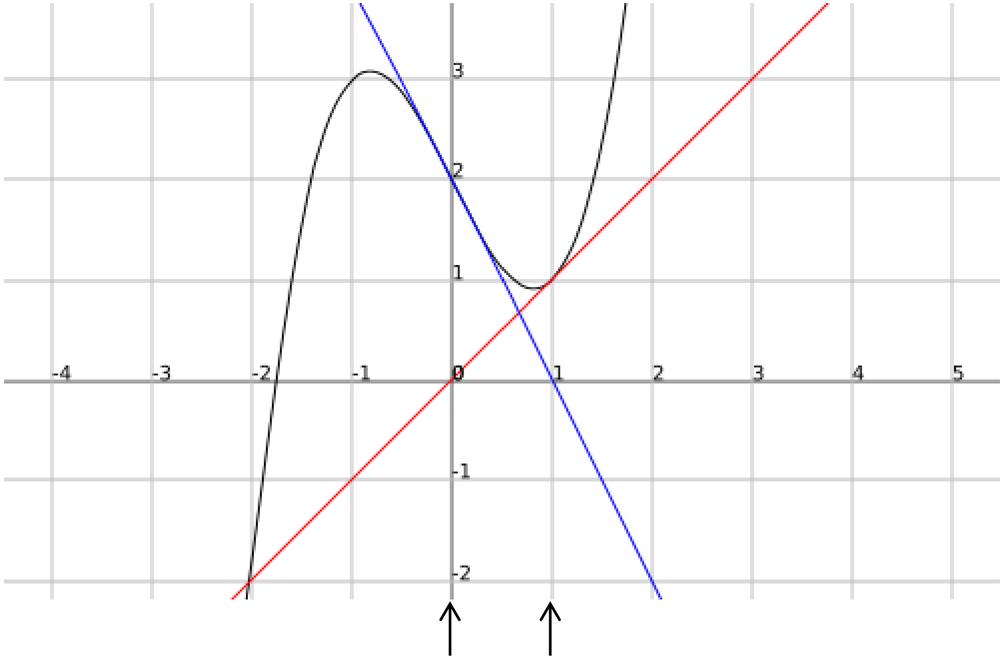


Derivative issues

1) No derivative at root
2) Discontinuous derivative
3) Zero derivative at root
4) No second derivative

Infinite Cycle

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



$x_0 = 0$ $x_1 = 1$

No Derivative

$$f(x) = \sqrt[3]{x}$$

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} = x_k - \frac{(x_k)^{1/3}}{1/3(x_k)^{-2/3}} = -2x_k$$

$$f(x) = |x|^{\gamma} \qquad 0 < \gamma \le 1/2$$

Discontinuous Derivative

$$f(x) = \begin{cases} 0 & x = 0 \\ x + x^2 \sin \dfrac{2}{x} & x \neq 0 \end{cases}$$

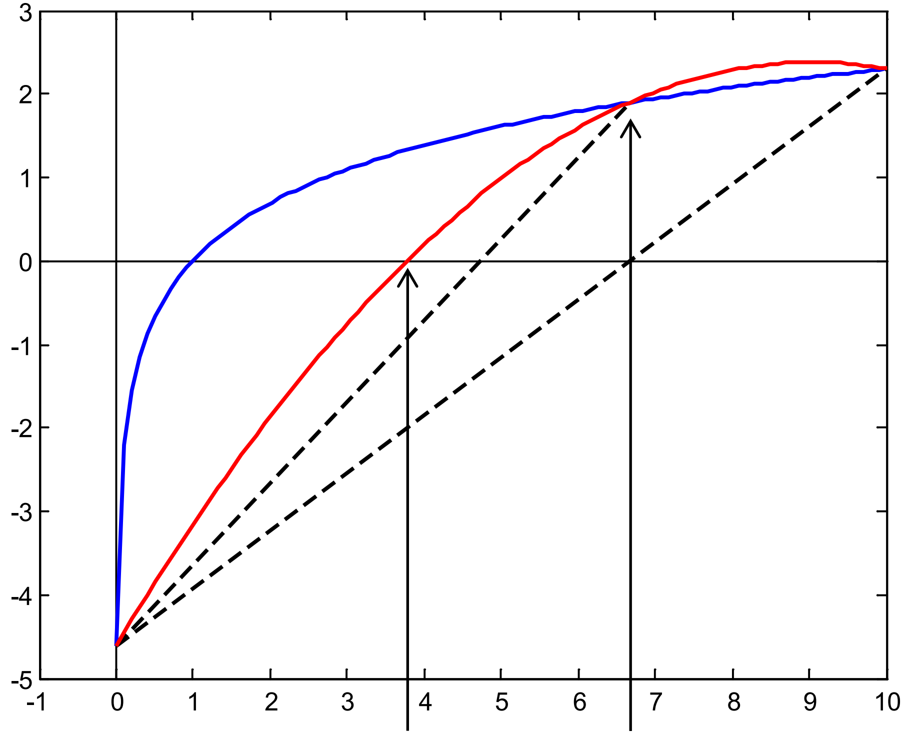
$$f'(x) = \begin{cases} 1 & x = 0 \\ 1 + 2x \sin \dfrac{2}{x} - 2\cos \dfrac{2}{x} & x \neq 0 \end{cases}$$

1) $f(x)$ is differentiable everywhere
2) $f(x)$ is infinitely differentiable, $x \neq 0$
3) $f'(0) \neq 0$
4) Derivative is bounded

However, Newton's method is divergent in any neighbourhood of the root!!

Inverse Quadratic Interpolation

$$f(x) = \log(x) = 0 \qquad x \in [0.01, \quad 10]$$



$x_0 = 0.01$ $\quad x_3$ $\quad x_2$ $\quad x_1 = 10$

Muller, Dekker, Brent

1) Muller, 1956: Inverse Quadratic Interpolation;
2) Dekker, 1969: Bisection + Secant;
3) Brent, 1973: Bisection + Secant + Quadratic

	Bisection	Secant	Muller's	Newton's
Order	$p = 1$	$p = 1.63$	$p = 1.84$	$p = 2$

$$p = \left(1+\sqrt{5}\right)\Big/2 \simeq 1.63 \qquad x^3 - x^2 - x - 1 = 0$$

Fixed Point Iterations

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} \equiv \phi(x_k)$$

$$x_{k+1} = \phi(x_k) \longrightarrow x = \phi(x)$$

Newton's method: $$\phi(x) = x - \frac{f(x)}{f'(x)}$$

$$0 = f(x) \longrightarrow x = x + f(x)$$

Convergence Theorem for FPI

1) $\phi: \left[a,b\right] \to \left[a,b\right]$

2) $\phi \in C^1\left[a,b\right]$

3) $\left|\phi'(x)\right| \le K < 1$

$\Longrightarrow$

1) $\exists^1 \ \alpha : \alpha = \phi(\alpha)$

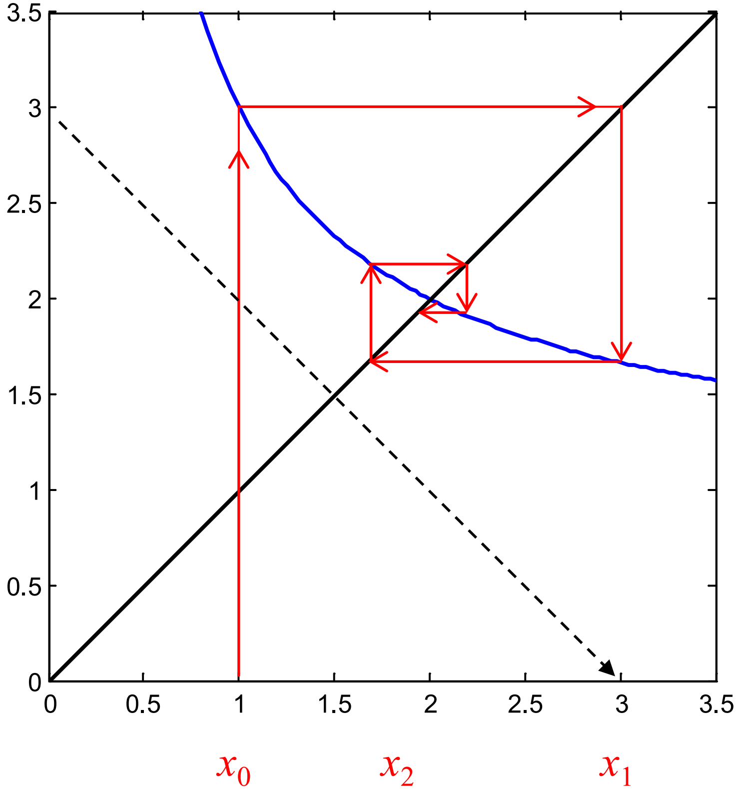
2) $x_k \xrightarrow[k\to\infty]{} \alpha$

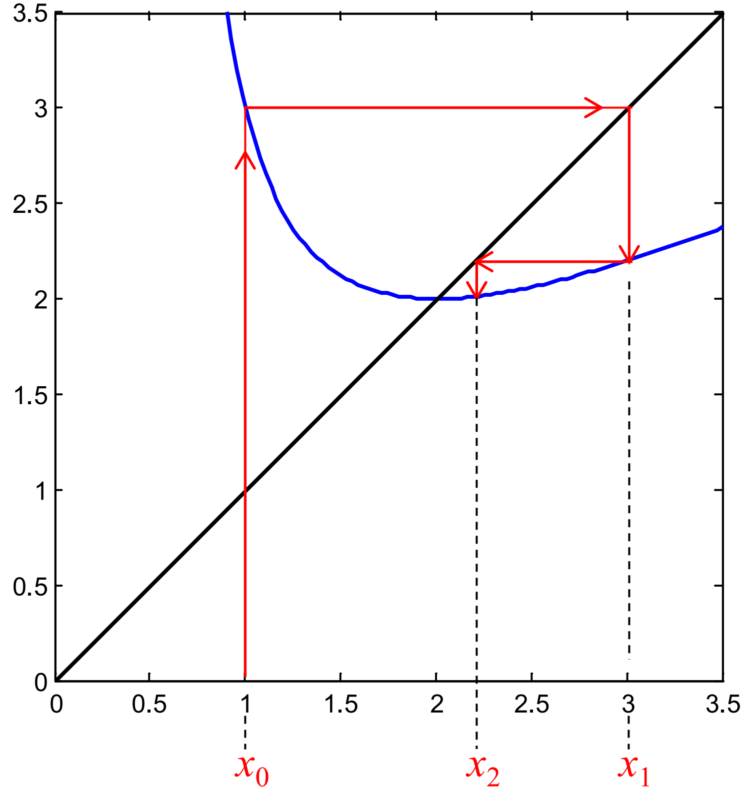
3) $\lim\limits_{k\to\infty} \dfrac{x_{k+1} - \alpha}{x_k - \alpha} = \phi'(\alpha)$

Example 1

$$f(x) = 1 + 2/x = x$$

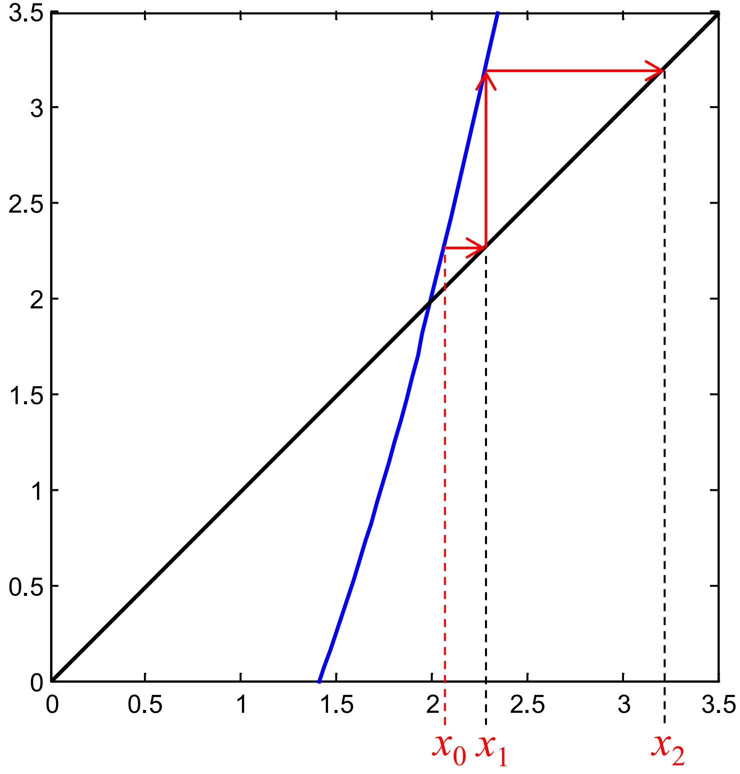
$$f(x) = \frac{x^2 + 2}{2x - 1} = x$$



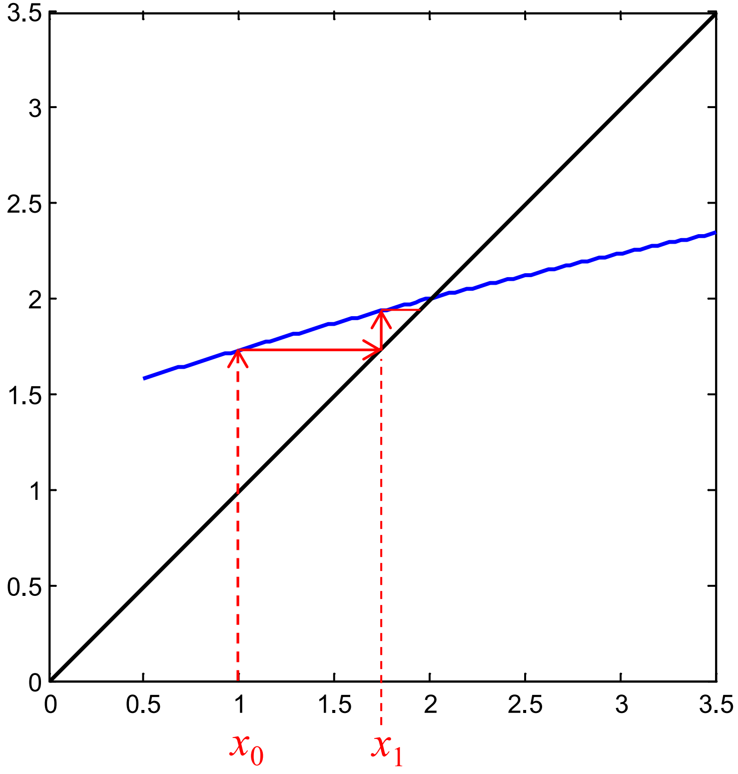


Example 2

$$f(x) = x^2 - 2 = x$$



$$f(x) = \sqrt{x+2} = x$$



Example 3

$$\cos x = \sin x$$

$$x + \cos x - \sin x = x$$

$$g(x) \equiv x + \cos x - \sin x$$

$$r = \pi/4 \approx 0.785398$$

$$|g'(r)| = |1 - \sqrt{2}| \approx 0.414$$

i	x_i	$g(x_i)$	$e_i = \lvert x_i - r\rvert$	e_i/e_{i-1}
0	0.0000000	1.0000000	0.7853982	
1	1.0000000	0.6988313	0.2146018	0.273
2	0.6988313	0.8211025	0.0865669	0.403
3	0.8211025	0.7706197	0.0357043	0.412
4	0.7706197	0.7915189	0.0147785	0.414
5	0.7915189	0.7828629	0.0061207	0.414
6	0.7828629	0.7864483	0.0025353	0.414
7	0.7864483	0.7849632	0.0010501	0.414
8	0.7849632	0.7855783	0.0004350	0.414
9	0.7855783	0.7853235	0.0001801	0.414
10	0.7853235	0.7854291	0.0000747	0.415
11	0.7854291	0.7853854	0.0000309	0.414
12	0.7853854	0.7854035	0.0000128	0.414
13	0.7854035	0.7853960	0.0000053	0.414
14	0.7853960	0.7853991	0.0000022	0.415
15	0.7853991	0.7853978	0.0000009	0.409
16	0.7853978	0.7853983	0.0000004	0.444
17	0.7853983	0.7853981	0.0000001	0.250
18	0.7853981	0.7853982	0.0000001	1.000
19	0.7853982	0.7853982	0.0000000	

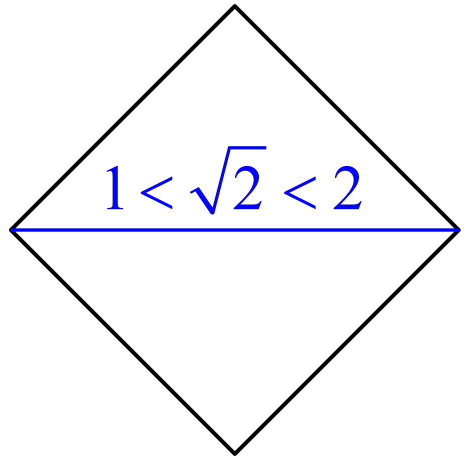
Concluding Remarks on FPI

- Necessary condition $\left|\phi'(\alpha)\right| < 1$
- Locally convergent
- Divergent when $\left|\phi'(\alpha)\right| > 1$
- It holds in vicinity of α $\left|x_{k+1} - \alpha\right| \approx \left|\phi'(\alpha)\right|\left|x_k - \alpha\right|$
- Quadratic convergence when $\phi'(\alpha) = 0$

Babylonian Algorithm

Tablet YBC7289

Around 1750 BC



$$a = 1 \qquad b = 2/a = 2$$

$$\sqrt{2} \approx \frac{1}{2}(a+b) = 1.5$$

$$x_0 = 1 \qquad x_{k+1} = \frac{1}{2}\left(x_k + \frac{2}{x_k}\right)$$

$$\sqrt{2} \approx x_2 = 1.41\overline{6}$$

$$x_{k+1} = \phi(x_k) \qquad \phi(x) \equiv \frac{1}{2}\left(x + \frac{2}{x}\right) \qquad \phi'(\sqrt{2}) = 0$$

Linear Convergence Control

$$x_{k+1} - \alpha \approx C\left(x_k - \alpha\right)$$

$$x_k - \alpha \approx C\left(x_{k-1} - \alpha\right)$$

$$x_{k+1} - x_k \approx C\left(x_k - x_{k-1}\right)$$

Iterate until $x_{k+1} - x_k \approx C\left(x_k - x_{k-1}\right)$

Evaluate $C \approx \left(x_{k+1} - x_k\right) / \left(x_k - x_{k-1}\right)$

Check: $-1 < C < 1$

$$\boxed{\begin{gathered} x_{k+1} - \alpha \approx C\left(x_k - \alpha\right) = C\left(x_k - x_{k+1} + x_{k+1} - \alpha\right) \\ \left(1 - C\right)\left(x_{k+1} - \alpha\right) \approx C\left(x_k - x_{k+1}\right) \\ \left(x_{k+1} - \alpha\right) \approx \frac{C}{1 - C}\left(x_k - x_{k+1}\right) \end{gathered}}$$

Stopping Criterion

$$\left(x_{k+1}-\alpha\right)\approx\frac{C}{1-C}\left(x_k-x_{k+1}\right)$$

Set SF such that $C'\equiv\frac{|C|}{1-C}SF\le 1$

Iterate until $C'\left|x_{k+1}-x_k\right|\le\varepsilon_{abs}$

$$\left|\frac{\alpha-x_{k+1}}{\alpha}\right|\approx\left|\frac{\alpha-x_{k+1}}{x_{k+1}}\right|\approx\frac{|C|}{1-C}\cdot\left|\frac{x_{k+1}-x_k}{x_{k+1}}\right|$$

Quadratic Conv. In Practice

- It is characterized by $\left|x_{k+1}-\alpha\right| \approx C\left|x_k-\alpha\right|^2$
- Rule of thumb 1:
  Number of correct digits doubles
- Use $x_k - x_{k-1}$ as convergence indicator
- Displacement is $\left|x_k - x_{k-1}\right| \approx \left|x_{k-1}-\alpha\right|$
- Rule of thumb 2:
  Number of leading zeros doubles in $\left|x_k - x_{k-1}\right|$

Important

- Scalar/Vector NLE
- Multiplicity
- Bracket
- Sensitivity/conditioning
- Bracketing vs. Open domain Methods
- Bisection, Secant, Newton’s, Muller’s
- Fixed Point Iterations, FPI