Methods to solve nonlinear equation(s) - Algebraic and transcendental

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Nonlinear equations - solution methods

1. Basic definitions/results
2. Numerical methods
   - Bisection method
   - Regula-Falsi Method (Method of false-position)
   - Newton's (Newton-Raphson) method
   - Secant method
   - Comparing through Examples
   - Fixed point iteration
3. Modified Newton's method - for multiple roots
4. Method for complex roots

- Our interest: Solve an equation of the form $f(x) = 0, \; x \in I \subset \mathbb{R}$

- Two types of f:
  - Algebraic: f is a polynomial
  - Transcendental: f is a function of elementary functions like $\sin, \cos, \log, x^a, e^x$, etc.
  - Examples: $x^5 - 2x^3 + 5x^2 + 2x + 1 = 0, \quad x - a\sin x = b$ (Kepler's eqn for planetary orbits), $\quad x^2 \log x + 2\sin 2x = 0$

- Iterative methods: Let $\alpha \in \mathbb{R}$ be such that $f(\alpha) = 0$. i.e., α is a root of $f(x) = 0$. Iterative methods are a class of methods to find α, which requires the knowledge of one or more initial guess values to start with. These methods produce a sequence of approximate values of α, say $\{x_k\}$.

- Order of convergence: A sequence of iterates $\{x_k | k \geq 0\}$ is said to converge to α with order $p \geq 1$, if

$$|\alpha - x_{k+1}| \leq C|\alpha - x_k|^p, \quad k \geq 0$$

  Here, $|\alpha - x_k| = e_k$, error at k^{th} iterative value with respect to actual solution and $C > 0$.
  Eg:- $p = 1$ (linear convergence), $p = 2$ (quadratic convergence).

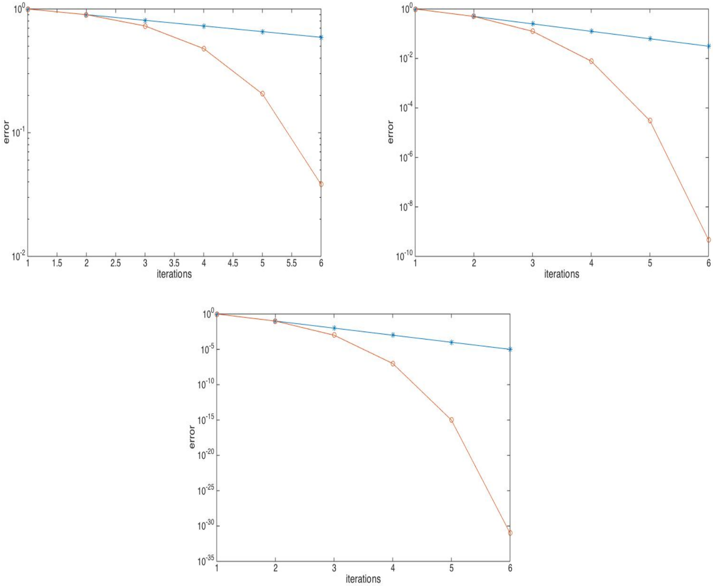

Figure: For $C = 0.9, 0.5, 0.1$ - Observe y-axis values to see the effect of C

- Stopping criteria: Provide an error tolerance ε (say 10^-6). Starting with initial guess x_0 (may be more initial guesses), $\{x_k\}_{k\geq 1}$ is evaluated till one or all of the following criteria are satisfied.
    - Absolute error check: $|x_{k+1} - x_k| < \varepsilon$
    - Relative error check: $\dfrac{|x_{k+1} - x_k|}{|x_k|} < \varepsilon$
    - Function value check: $|f(x_{k+1})| < \varepsilon$
- Recall: Intermediate value theorem, mean value theorem, finding maxima & minima of f in an interval, Taylor series expansion etc.

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- Assumption: f is continuous on $[a, b]$.

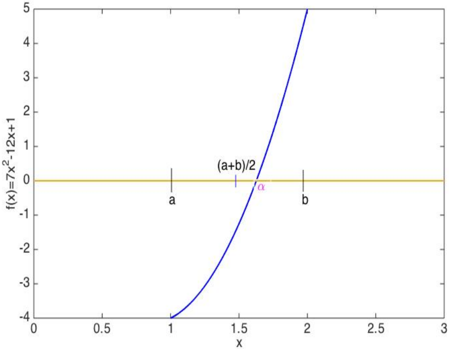

Figure: Bisection method

Algorithm:

1. Choose tolerance values $\varepsilon, \delta > 0$. Fix $[a_0, b_0] \subset [a, b]$ so that $f(a_0)f(b_0) < 0$
2. Evaluate $c = \frac{a_0+b_0}{2}$.
3. IF $|f(c)| \leq \varepsilon$ and $|c - a_0| < \delta$, STOP

   ELSE "If $f(a_0)f(c) < 0$ then $b_0 = c$ elseif $f(b_0)f(c) < 0$ then $a_0 = c$," and repeat step 2.

- Is it possible for all continuous functions to do bracketing? NO! Eg: x^2

Required number of iterations for desired accuracy:

- Length of starting interval $b_0 - a_0$
- Length of the interval at k^{th} iteration: $\frac{b_0 - a_0}{2^k}$
- Difference between a_k (or) b_k and $c_k = \frac{a_k + b_k}{2}$ is $\frac{b_0 - a_0}{2^{k+1}}$
- Iteration stops when $\frac{b_0 - a_0}{2^{k+1}} < \varepsilon \implies k > \frac{\log |b_0 - a_0| - \log \varepsilon}{\log 2}$ (ignored the condition on f)

Outline

- Assumption: f is continuous on $[a, b]$.

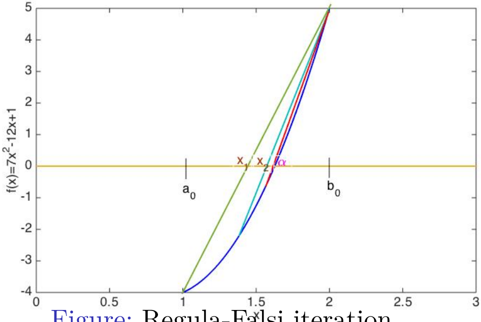

Figure: Regula-Falsi iteration

- At each iteration: The point x_k is calculated by approximating f with the chord connecting $(a_k, f(a_k))$ and $(b_k, f(b_k))$.
- Eqn of the st. line: $\dfrac{y - f(a_k)}{x - a_k} = \dfrac{f(b_k) - f(a_k)}{b_k - a_k}$.
- Intersection of the above st. line with $x - axis$ gives $x_k = \dfrac{a_k f(b_k) - b_k f(a_k)}{f(b_k) - f(a_k)}$.

- Algorithm:
  For $k = 0, 1, 2, \cdots$
  1. Choose tolerance values $\varepsilon, \delta > 0$. Fix $[a_k, b_k] \subset [a, b]$ so that $f(a_k)f(b_k) < 0$
  2. Evaluate $c = \dfrac{a_k f(b_k) - b_k f(a_k)}{f(b_k) - f(a_k)}$.
  3. IF $|f(c)| \leq \varepsilon$ and $|c - a_k| < \delta$, STOP

     ELSE
     $k = k + 1$
     "if $f(a_k)f(c) < 0$ then $a_k = a_k,\ b_k = c$ elseif $f(b_k)f(c) < 0$ then $a_k = c,\ b_k = b_k$" and repeat step 2.

Outline

- Assumption: f is twice continuously differentiable on $[a, b]$. f, f' are continuous and f'' exists in $[a, b]$.
- Derivation: Let x_0 be an initial guess for α (true root) so that $f'(x_0) \neq 0$ and $|x_0 - \alpha|$ is "small" enough.
  Since α is a root, $$f(\alpha) = 0 \tag{1}$$
  Using Taylor expansion,

$$0 = f(\alpha) = f(x_0 + \alpha - x_0) = f(x_0) + (\alpha - x_0) f'(x_0) + \frac{(\alpha - x_0)^2}{2!} f''(\xi)$$

where ξ lies between x_0 and α.

Ignoring $(\alpha - x_0)^2$ and higher order terms (since $\alpha - x_0$ is small enough),

$$0 \approx f(x_0) + (\alpha - x_0) f'(x_0) \implies \alpha \approx x_0 - \frac{f(x_0)}{f'(x_0)} \tag{2}$$

Taking $x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$ (since x_0 is only an approximation) and proceed as in above steps, we obtain $x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$.
Hence, repeating the steps k times, we obtain an iterative formula

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, \quad k \geq 0, \quad f'(x_k) \neq 0 \tag{3}$$

- Geometrical meaning: Let x_0 be the initial value for the Newton-Raphson method (iteration) for the root of $f(x) = 0$
  Eqn of the tangent of f at x_0 is $y - f(x_0) = f'(x_0)(x - x_0)$

  To get the $x - \textit{intercept}$ of the tangent line, put $y = 0$

  $$\Rightarrow \quad 0 - f(x_0) = f'(x_0)(x^* - x_0) \quad \Rightarrow \quad x^* = x_0 - \frac{f(x_0)}{f'(x_0)}$$

  i.e., x_1 is the $x - \textit{intercept}$ of the tangent of f at $(x_0, f(x_0))$, x_2 is the $x - \textit{intercept}$ of the tangent of f at $(x_1, f(x_1))$ and so on.

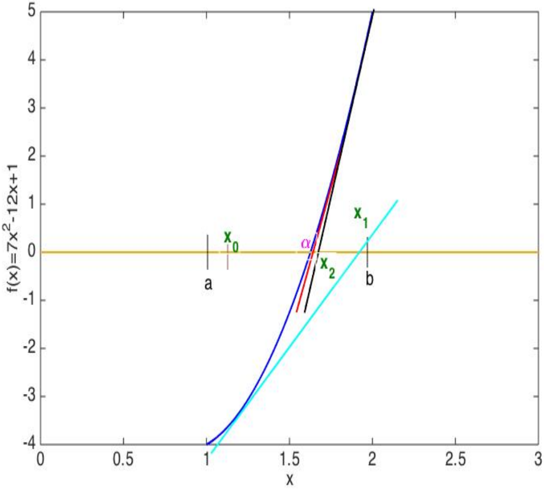

Figure: Newton-Raphson iteration

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- Assumption: f is twice continuously differentiable on $[a, b]$. f, f' are continuous and f'' exists in $[a, b]$.
- Secant method: In Newton's method, replace $f'(x_k)$ with finite difference approximate formulae $f'(x_k) = \dfrac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}$
- Formula: $x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})}$
- Formula is same as Regula-Falsi method (method of false position).
- Regula-Falsi method: Bracketing of the root is ensured at each iteration.

  Secant method: Does not ensure bracketing of the root.

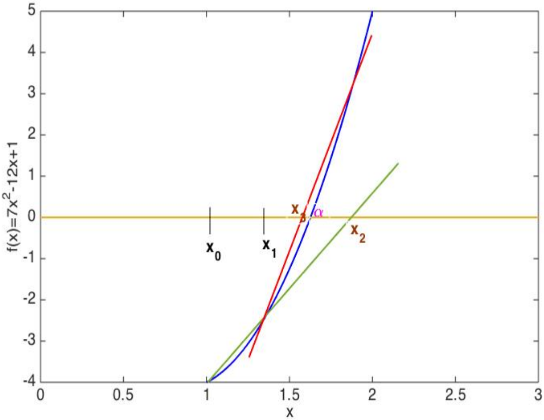


Figure: Secant iteration

Outline

- Example: $f(x) = \cos(x) - xe^x$. Find a zero of f in the interval $[0, 1]$.
- $a_0 = 0,\ b_0 = 1,\ \ f(a_0) = 1 > 0,\ \ f(b_0) = \cos(1) - e < 0$. Hence by IVT, there exists a root for $f(x) = 0$ in $[0, 1]$.
- $\varepsilon = \delta = 1e - 03$, Calculations by rounding off values at each iteration to 4 decimal places.

Table: Bisection iteration

k	a_k	b_k	$c_k = \frac{a_k+b_k}{2}$	$f(c_k)$
0	0.0000	1.0000	0.5000	0.0532
1	0.5000	1.0000	0.7500	-0.8561
2	0.5000	0.7500	0.6250	-0.3567
3	0.5000	0.6250	0.5625	-0.1413
4	0.5000	0.5625	0.5313	-0.0417
5	0.5000	0.5313	0.5156	0.0066
6	0.5156	0.5313	0.5235	-0.0176
7	0.5156	0.5235	0.5196	-0.0056
8	0.5156	0.5196	0.5176	0.0005
9	0.5176	0.5196	0.5186	-0.0026
10	0.5176	0.5186	0.5181	-0.0010

Table: Regula-falsi iteration

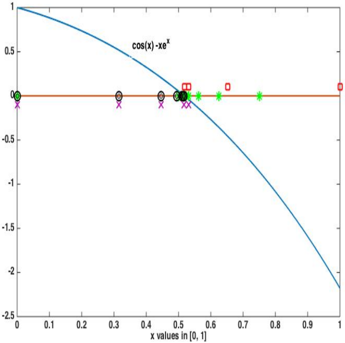
k	a_k	b_k	$c_k = \frac{a_k f(b_k) - b_k f(a_k)}{f(b_k) - f(a_k)}$	$f(c_k)$
0	0	1.0000	0.3147	0.5198
1	0.3147	1.0000	0.4467	0.2036
2	0.4467	1.0000	0.4940	0.0708
3	0.4940	1.0000	0.5099	0.0237
4	0.5099	1.0000	0.5152	0.0078
5	0.5152	1.0000	0.5169	0.0026
6	0.5169	1.0000	0.5175	0.0008

Table: Newton-Raphson iteration

k	$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$	$f(x_{k+1})$
0	1.0000	-2.1780
1	0.6531	-0.4607
2	0.5314	-0.0420.
3	0.5179	-0.0004.
4	0.5178	-0.0001.

Table: Secant iteration

k	a_k	b_k	$c_k = \frac{a_k f(b_k) - b_k f(a_k)}{f(b_k) - f(a_k)}$	$f(c_k)$
0	0	1.0000	0.3147	0.5198
1	1.0000	0.3147	0.4467	0.2036
2	0.3147	0.4467	0.5317	-0.0429
3	0.4467	0.5317	0.5169	0.0026
4	0.5317	0.5169	0.5177	0.0002



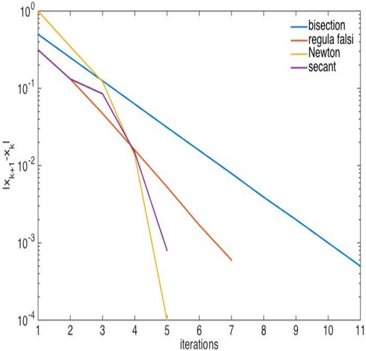


Figure: Fig 1: green(*) - bisection, black(o) - Regula falsi, red - Newton, magenta - Secant iterate values, Fig 2: Convergence of the iterates for all methods

- Example 2: $f(x) = x^3$. Find a zero of f in the interval $[0, 1]$.
- $a_0 = -1,\ b_0 = 0.5,\quad f(a_0) = -1 < 0,\quad f(b_0) = 0.125 > 0$. Hence by IVT, there exists a root for $f(x) = 0$ in $[-1, 0.5]$.
- $\varepsilon = \delta = 1e - 03$, Calculations by rounding off values at each iteration to 4 decimal places

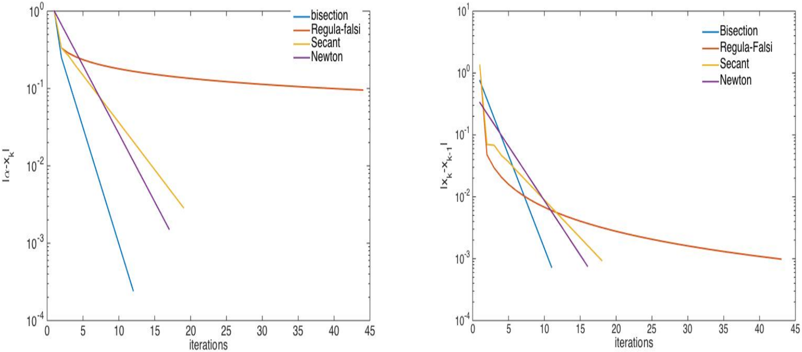


Figure: Convergence of the iterates for all methods - Observe linear convergence of Newton-Raphson method

Outline

- Definition: The number p is called a fixed point of a function g, if $g(p) = p$. i.e., p is a point on the $x-$axis, where graphs of $y = g(x)$ and $y = x$ intersect.
  Eg: Fixed points of $\sin x$ are points that satisfy the equation $\sin x = x$.
- Relevance to root finding: Given a root finding problem, $f(x) = 0$, we can define functions g (using f), which has a fixed point α (root of $f(x) = 0$). i.e., $g(\alpha) = \alpha$.
- For a given f, g is not unique (so that $g(\alpha) = \alpha$.
  Eg-1: For $f(x)$, $g_1(x) = x - f(x)$ and $g_2(x) = x + af(x), \quad a \neq 0$ (are just two choices of g).
  Eg-2: $f(x) = x^2 - c, \quad c > 0 \Rightarrow g_1(x) = x + a(x^2 - c), \quad a \neq 0$, $g_2(x) = c/x$, $g_3(x) = \frac{1}{2}(x + \frac{c}{x})$, $g_4(x) = x - \frac{x^2 - c}{2x}$

- Theorem: - (Existence and uniqueness of a fixed point)
  (i) If g is continuous in $[a,b]$ and $g([a,b]) \subseteq [a,b]$, then g has at least one fixed point in $[a,b]$.
  (ii) If, in addition, $g'(x)$ exists on (a,b) and a positive constant $K<1$ exists with $|g'(x)| \leq K < 1, \forall\ x \in (a,b)$
  Then there exists exactly one fixed point in $[a,b]$.
- Eg: $g(x) = x^2/3$ and $[a,b]=[0,1]$. $\implies g([0,1]) = [0,1/3] \subset [0,1]$ and $|g'(x)| = 2x/3 < 1, \ \ \forall\ x \in (0,1)$. Fixed point $p=0$.
- Above theorem is sufficient, not necessary condition. Eg: $g(x) = \frac{1}{3^x}$. Clearly $g([0,1]) = [1/3,1] \subset [0,1]$. Hence there exists at least one fixed point. But $g'(x) = \frac{\log 3}{3^x} \geq 1$ in $(0, \frac{\log(\log 3)}{2\log 3})$ (verify!). Still g has unique fixed point in $[0,1]$. (Next figure).

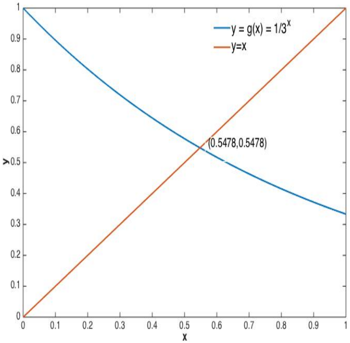


Figure: Fixed point of $g(x) = \frac{1}{3^x}$

- Fixed point iteration method: To find the root of $f(x) = 0$.
  Step 1. Rewrite $f(x) = 0$ in the form $g(x) = x$.
  Step 2. Starting with an initial approximate x_0 for α, we obtain $\{x_k\}$ using the formula $x_{k+1} = g(x_k), \quad k \geq 0$

- The question: For the function f, how to choose g (Among all possible g for f) so that the sequence $\{x_k\}$ converges to the root of $f(x) = 0$ (i.e., α)? There are two issues: (i) $\{x_k\}$ can diverge OR (ii) $\{x_k\}$ converges, but not to α.

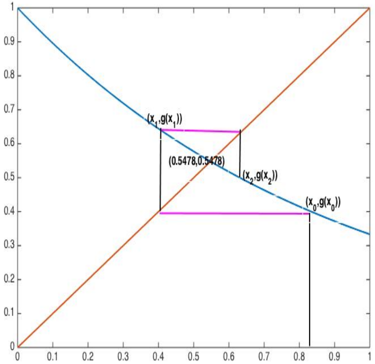
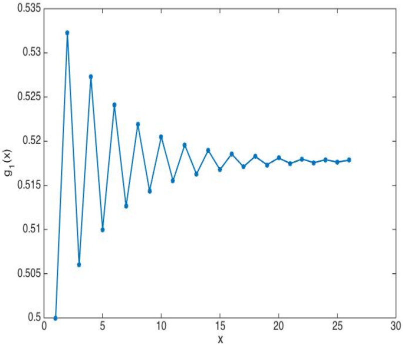
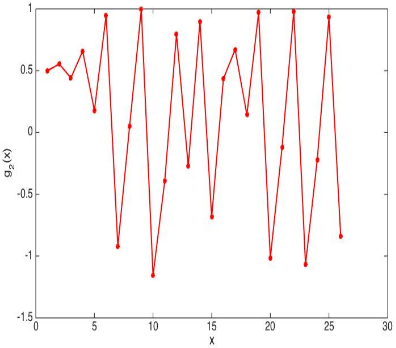


Figure: Fixed point iteration

- Example: $f(x) = \cos x - xe^x$ in $[0,1]$. Choose $x_0 = 0.5$ and $\alpha = 0.5176$
  (1) $g_1(x) = e^{-x}\cos x$ (2) $g_2(x) = x + \cos x - xe^x$
  (3)$g_3(x) = \log(\frac{\cos x}{x})$ (4) $g_4(x) = x - \dfrac{\cos x - xe^x}{-\sin x - (x+1)e^x}$





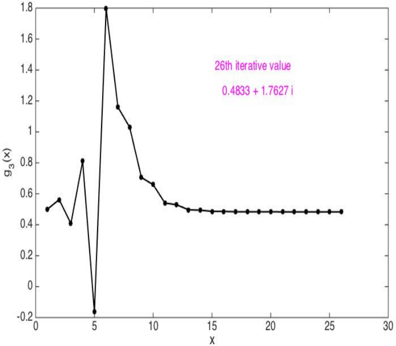


Figure: Fixed point iteration using (i) $g_1(x)$, (ii) $g_2(x)$, (iii) $g_3(x)$ - What about g_4?

- Fixed point theorem: Let g is continuous on $[a,b]$ and $g([a,b]) \subseteqq [a,b]$. Suppose, in addition, $g'(x)$ exists on (a,b) and a a constant $0 < K < 1$ exists with $|g'(x)| \leq K < 1, \forall\ x \in (a,b)$. Then for any $x_0 \in [a,b]$, the sequence defined by $x_{k+1} = g(x_k),\ k \geq 1$ converges to a unique fixed point α in $[a,b]$.

  Proof: Prove that (i) g has a unique fixed point α in $[a,b]$.
  (ii) $\{x_k\}$ generated by $x_{k+1} = g(x_k),\ k \geq 0$ coverges to this fixed point.
  Using existence and uniqueness theorem g has a unique fixed point in $[a,b]$, say α

$$g(\alpha) = \alpha \tag{1}$$

Since g maps $[a,b]$ into itself, $x_k \in [a,b], \quad k = 0,1,2,\ldots$ Also $|g'(x)| \leq K < 1$. Hence (using above inequality and LMVT)

$$\begin{aligned} |x_k - \alpha| &= |g(x_{k-1}) - g(\alpha)| && (2) \\ &= |g'(\xi_k)||x_{k-1} - \alpha|, \quad \xi_k \text{ lies between } x_{k-1} \text{ \& } \alpha && (3) \\ &\leq K|x_{k-1} - \alpha| && (4) \end{aligned}$$

Inequality (4) implies order convergence is *at least* linear.

Applying above inequality recursively, we get,

$|x_k - \alpha| \leq K|x_{k-1} - \alpha| \leq K^2|x_{k-2} - \alpha| \leq \ldots\ldots \leq K^k|x_0 - \alpha|$

Since $0 < K < 1$, $\lim\limits_{k\to\infty} K^k = 0$. Hence

$$\lim_{k\to\infty} |x_k - \alpha| \leq \lim_{k\to\infty} K^k|x_0 - \alpha| = 0$$

$$\implies \quad \lim_{k\to\infty} |x_k - \alpha| = 0 \quad \implies \quad x_k \to \alpha \text{ as } k \to \infty$$

This proves that $\{x_k\}$ converges to fixed point of g in $[a,b]$.

- Remark: If all the assumptions in the above theorem are satisfied, then the bounds of the error at k^{th} iteration $|x_k - \alpha|$ is given by

$$|x_k - \alpha| \leq K^k \max\{x_0 - a, b - x_0\} \quad (5)$$

$$|x_k - \alpha| \leq \frac{K}{1-K}|x_k - x_{k-1}| \quad (6)$$

$$|x_k - \alpha| \leq \frac{K^k}{1-K}|x_1 - x_0| \quad (7)$$

Proof: (1) From previous theorem,
$|x_k - \alpha| \leq K^k |x_0 - \alpha| \leq K^k \max\{x_0 - a, b - x_0\}$

(2) & (3) Consider

$$
\begin{aligned}
|x_k - x_{k-1}| &= |g(x_{k-1}) - g(x_{k-2})| && (8)\\
&= |g'(\xi_{k-1})||x_k - x_{k-1}| && (9)\\
&\leq K|x_{k-1} - x_{k-2}| && (10)\\
&\vdots && (11)\\
&\leq K^{k-1}|x_1 - x_0| && (12)
\end{aligned}
$$

Now

$$
\begin{aligned}
|\alpha - x_k| &= |g(\alpha) - g(x_{k-1})| && (13)\\
&= |g'(\xi_k)||\alpha - x_{k-1}| && (14)\\
&\leq K|\alpha - x_{k-1}| && (15)\\
&= K|\alpha - x_k + x_k - x_{k-1}| && (16)\\
&\leq K|\alpha - x_k| + K|x_k - x_{k-1}| && (17)\\
\text{i.e., } |\alpha - x_k| &\leq \frac{K}{1-K}|x_k - x_{k-1}| && (18)\\
\text{i.e., } |\alpha - x_k| &\leq \frac{K}{1-K}K^{k-1}|x_1 - x_0| = \frac{K^k}{1-K}|x_1 - x_0| && (19)
\end{aligned}
$$

- Note: Above inequalities show that the rate at which $\{x_k\}$ converges to α depends on K, the bound for $g'(x)$ in $[a, b]$. i.e., The smaller the value of K, faster the convergence. If K is close to **one**, convergence would be very slow.

- Example 1: Use fixed point iteration to find a positive root between 0 and 1 of the equation $xe^x = 1$.
  Here $f(x) = 1 - xe^x$. Rewriting let $x = e^{-x}$. Hence one choice of $g(x) = e^{-x}$

  Is it a good choice? $g'(x) = -e^{-x}$ and $\max_{(0,1)}|g'(x)| < 1$ (why? Also what is the value of K ?)

  Iterates: 1.0000 0.3679 0.6922 0.5005 0.6062 0.5454 0.5796 0.5601 0.5711 0.5649 0.5684 0.5664 0.5676 0.5669 0.5673 0.5671 0.5672 0.5671 0.5672 0.5671 0.5671

- Example 2: Find the real root of $x^3 + x^2 - 1 = 0$ on the interval $[0, 1]$ with an accuracy of 10^{-4} with respect to α for the choice $g(x) = \frac{1}{\sqrt{1+x}}$.(Discussed in the class!).

- Convergence of Newton's method: This theorem establishes the condition for convergence and order of convergence on Newton-Raphson method. Following theorem ensures only local convergence for Newton's method

  Statement: Let f and f' are differentiable in $[a, b]$ and f'' is continuous on $[a, b]$. Also let, for $\alpha \in (a, b)$, $f(\alpha) = 0$ and $f'(\alpha) \neq 0$. Then there exists a $\delta > 0$ so that Newton's (Newton-Raphson) method generates a sequence $\{x_k\}$ converging to α for any initial approximation x_0 chosen from $(\alpha - \delta, \alpha + \delta)$. Also $\{x_k\}$ converges to α **quadratically**.

  Proof: From Newton's formula, $g = x - \frac{f(x)}{f'(x)}$.
  To Prove: (1) $\exists$ an interval $(\alpha - \delta, \alpha + \delta)$ so that g maps into itself. (So that fixed point iteration converges)
  (2) $\exists$ a K such that $0 < K < 1$ & $|g'(x)| \leq K, \quad \forall x \in (\alpha - \delta, \alpha + \delta)$

From the assumptions, since f' is continuous on $[a, b]$ and $f'(\alpha) \neq 0$, by sign preserving property of continuous functions

$$f'(x) \neq 0, \quad \forall\, x \in [\alpha - \delta_1, \alpha + \delta_1)] \subseteqq [a, b], \quad \text{for some } \delta_1 > 0$$

Also

$$g'(x) = 1 - \frac{f'(x)^2 - f(x)f''(x)}{f'(x)^2} = \frac{f(x)f''(x)}{f'(x)^2}, \text{ for } x \in [\alpha - \delta_1, \alpha + \delta_1]$$

$$f \in C^2[\alpha - \delta_1, \alpha + \delta_1] \; (\because [\alpha - \delta_1, \alpha + \delta_1]) \implies g \in C^2[\alpha - \delta_1, \alpha + \delta_1]$$

Also $g'(\alpha) = \frac{f(\alpha)f''(\alpha)}{f'(\alpha)^2} = 0 \quad (\because f(\alpha) = 0)$

Hence

$$g'(x) \in C[\alpha - \delta_1, \alpha + \delta_1] \;\&\; g'(\alpha) = 0 \implies \text{for any } 0 < K < 1, \; \exists \delta \leq \delta_1$$

so that

$$|g'(x)| < K, \quad \forall x \in (\alpha - \delta, \alpha + \delta)$$

TST g maps $[\alpha-\delta, \alpha+\delta]$ onto itself. For $x \in [\alpha-\delta, \alpha+\delta]$

$$\begin{aligned} |g(x)-\alpha| &= |g(x)-g(\alpha)| && (20)\\ &= |g'(\xi)||x-\alpha|, \xi \text{ lies between } x \text{and} \alpha && (21)\\ &\leq K|x-\alpha| && (22)\\ &< |x-\alpha| && (23)\end{aligned}$$

Therefore $|x-\alpha| < \delta \implies |g(x)-\alpha| < \delta$.
Consequently $g([\alpha-\delta, \alpha+\delta]) \subseteqq [\alpha-\delta, \alpha+\delta]$
All requirements of fixed point theorem is satisfied. Hence $\{x_k\}$ with $x_0 \in (\alpha-\delta, \alpha+\delta)$ defined by

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, \quad k \geq 0$$

converges to α.

Order of convergence: Let $e_k = x_k - \alpha$. Also given that $f'(\alpha) \neq 0$

$$\begin{aligned} e_{k+1} &= x_{k+1} - \alpha && (24)\\ &= x_k - \frac{f(x_k)}{f'(x_k)} - \alpha && (25)\\ &= e_k - \frac{f(x_k)}{f'(x_k)} && (26)\\ &= \frac{e_k f'(x_k) - f(x_k)}{f'(x_k)} && (27) \end{aligned}$$

Since α is the root,

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

where ξ_k lies between α and x_k

$$\text{i.e.,} \quad e_k f'(x_k) - f(x_k) = \frac{e_k^2}{2!} f''(\xi_k)$$

$$\text{Then} \quad e_{k+1} = \frac{e_k f'(x_k) - f(x_k)}{f'(x_k)} = \frac{e_k^2 f''(\xi_k)}{2\ f'(x_k)}$$

$$e_{k+1} \approx \frac{e_k^2 f''(r)}{2\ f'(r)} = Ce_k^2, \quad \text{where} \ \ \xi_k \approx x_k (= r)$$

Hence Newton-Raphson method converges quadratically, if $x_0 \in (\alpha - \delta, \alpha + \delta)$.

- Definition: A number α is said to be a root of multiplicity m for the equation $f(x) = 0$, if for $x \neq \alpha$, we can write $f(x) = (x - \alpha)^m q(x)$, where $\lim_{x \to \alpha} q(x) \neq 0$.

- Theorem: A differentiable function f in $[a, b]$ has a simple zero α in $[a, b]$, if and only if, $f(\alpha) = 0$ and $f'(\alpha) \neq 0$.

- Theorem: A function $f \in C^m[a, b]$ has a zero α of multiplicity m in $[a, b]$, if and only if, $f(\alpha) = f'(\alpha) = \cdots\cdots = f^{(m-1)}(\alpha) = 0, \text{ but } f^{(m)}(\alpha) \neq 0$.

- Newton's method for multiple roots: Let α be a root of multiplicity m. Consider the function

$$
\begin{aligned}
h(x) &= \frac{f(x)}{f'(x)} && (28) \\
\text{Also we have, } f(x) &= (x-\alpha)^m q(x), \quad q(\alpha) \neq 0 && (29) \\
\text{Then, } h(x) &= \frac{(x-\alpha)^m q(x)}{m(x-\alpha)^{m-1} q(x) + (x-\alpha)^m q'(x)} && (30) \\
&= \frac{(x-\alpha) q(x)}{m q(x) + (x-\alpha) q'(x)} && (31) \\
&= (x-\alpha)\left(\frac{q(x)}{m q(x) + (x-\alpha) q'(x)}\right) && (32)
\end{aligned}
$$

Clearly α is a root for $h(x) = 0$. Also it is a simple root because,

$$
\frac{q(\alpha)}{m q(\alpha) + (\alpha-\alpha) q'(\alpha)} = \frac{1}{m} \neq 0
$$

- Newton-Raphson method for h: Applying Newton-Raphson to $h(x) = 0$ gives

$$
\begin{aligned}
x_{k+1} &= x_k - \frac{h(x_k)}{h'(x_k)} && (33)\\
&= x_k - \frac{f(x_k)/f'(x_k)}{[f'(x_k)^2 - f(x_k)f''(x_k)]/f'(x_k)^2} && (34)\\
x_{k+1} &= x_k - \frac{f(x_k)f'(x_k)}{[f'(x_k)^2 - f(x_k)f''(x_k)]} && (35)
\end{aligned}
$$

- Note: If $g(x) = x - \frac{h(x)}{h'(x)}$ satisfy required continuity and differentiability conditions, the iteration converges quadratically, regardless of the multiplicity of the root of $f(x) = 0$.

  Caution - Drawback is that this formula is that it can cause serious round-off issues as the denominator is the difference of two numbers ($f(x_k)$, $f'(x_k)$ at least) that are close to zero.

- Example 1: $f(x) = x^3, \quad \delta = \varepsilon = 10^{-06}, \quad x_0 = -1$

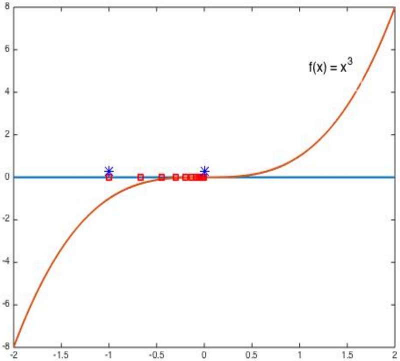
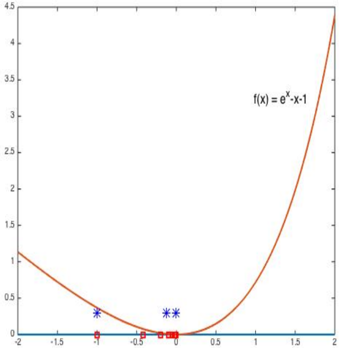


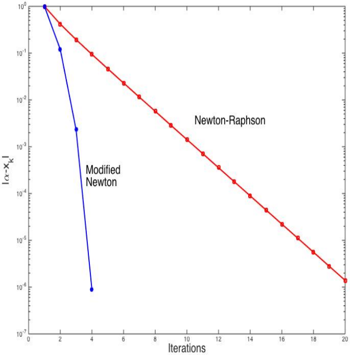
Figure: Iterates of Newton (red $\square$) and modified Newton methods (blue $*$)

- However, modified Newton's method faces an issue for this example! Any guess?

- Example 2: $f(x) = e^x - x - 1, \quad \delta = \varepsilon = 10^{-06}, \quad x_0 = -1$



(i)



(ii)

Figure: (i) Iterates and (ii) order of convergence - of Newton and modified Newton methods.

- **Modified Newton's method (Alternate formula)**
  1. If α is root of multiplicity m, then error at $(k+1)^{th}$ iteration for Newton's method (Not modified method's!) is

  $$e_{k+1} \approx \left(1 - \frac{1}{m}\right)e_k + \frac{1}{m^2(m+1)}\frac{f^{(m+1)}(\alpha)}{f^{(m)}(\alpha)}e_k^2 + O(e_k^3)$$

  This relation says Newton's method converge only linearly when $m > 1$!
  2. Consider the formula $x_{k+1} = x_k - a\frac{f(x_k)}{f'(x_k)}, \quad a \in \mathbb{R}$
  3. Error for above formula:

  $$e_{k+1} \approx \left(1 - \frac{a}{m}\right)e_k + \frac{a}{m^2(m+1)}\frac{f^{(m+1)}(\alpha)}{f^{(m)}(\alpha)}e_k^2 + O(e_k^3)$$

  4. Above error relation implies modified formula $x_{k+1} = x_k - m\frac{f(x_k)}{f'(x_k)}$ gives quadratic convergence. (Solve above example using this formula)
  5. But... Formula is useful only if multiplicity m is known a priori!

Muller's method

- All the methods discussed so far ensures that subsequent iterates are real, provided initial guess(es) is/are real numbers.
- But what about a polynomial equation having real coefficients, but complex roots?
- Exercise: Check if Newton's method iterates to a complex root, if x_0 is complex. Possible with complex arithmetic.
- We are going to look at an alternate method: Muller's method

Muller's method

Theorem 1

If $z = a + bi$ is a complex zero of multiplicity m of the polynomial $P(x)$ with real coefficients, then $z = a - bi$ is also a zero of multiplicity m of the polynomial $P(x)$, and $(x^2 - 2ax + a^2 + b^2)^m$ is a factor of $P(x)$.

- Muller's method is applicable to any root finding problem, but particularly useful in finding the roots of polynomials.
- At each iteration Muller's method approximates function f with a parabola passing through $(x_{k-1}, f(x_{k-1})), (x_k, f(x_k)), (x_{k+1}, f(x_{k+1}))$.

Muller's method

- $P(x) = a(x - x_2)^2 + b(x - x_2) + c$
- $P(x_0) = f(x_0) \implies a(x_0 - x_2)^2 + b(x_0 - x_2) + c = f(x_0)$
- $P(x_1) = f(x_1) \implies a(x_1 - x_2)^2 + b(x_1 - x_2) + c = f(x_1)$
- $P(x_2) = f(x_2) \implies c = f(x_2)$

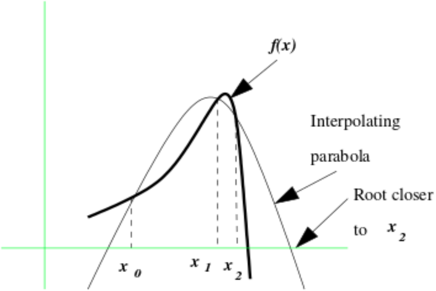


Figure: Muller's method

Muller's method

Then solving for $a, b, c,$ we get

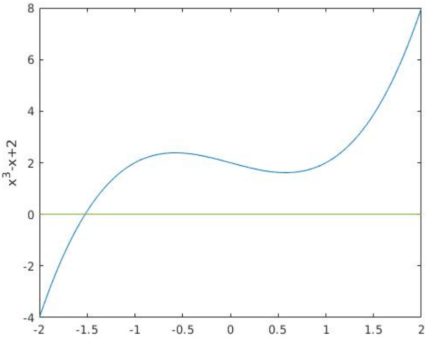
- $c = f(x_2)$
- $b = \frac{(x_0-x_2)^2[f(x_1)-f(x_2)]-(x_1-x_2)^2[f(x_0)-f(x_2)]}{(x_0-x_2)(x_1-x_2)(x_0-x_1)}$
- $a = \frac{(x_1-x_2)[f(x_0)-f(x_2)]-(x_0-x_2)[f(x_1)-f(x_2)]}{(x_0-x_2)(x_1-x_2)(x_0-x_1)}$

Next iterate is calculated as

- $x_3 - x_2 = \frac{-2c}{b \pm \sqrt{b^2-4ac}}$
- Muller's method: $x_3 = x_2 + \frac{-2c}{b + sign(b)\sqrt{b^2-4ac}}$

Muller's method

Example: Find the roots of $f(x) = x^3 - x + 2$ using Muller's method.



Muller's method

Table: Muller's method iteration: Initial guesses - $0, -0.5, -1$

x(1) = -1.75830573921179 - 0.00000000000000i
x(2) = -1.48746280049662 - 0.00000000000000i
x(3) = -1.51942498221994 - 0.00000000000000i
x(4) = -1.52139683387808 - 0.00000000000000i
x(5) = -1.52137969823106 - 0.00000000000000i
x(6) = -1.52137970680453 - 0.00000000000000i
x(7) = -1.52137970680457 - 0.00000000000000i
x(8) = -1.52137970680457 - 0.00000000000000i

Muller's method

Table: Muller's method iteration: Initial guesses - $0.5 + i, 0.5 + 0.9i, 0.5 + 0.8i$

x(1) = 0.73687784183239 + 0.99947379832872i
x(2) = 0.83889379452510 + 0.86179624331771i
x(3) = 0.76558290827779 + 0.80182809773579i
x(4) = 0.71859106526626 + 0.85190248742136i
x(5) = 0.75720478527562 + 0.88636185266192i
⋮
x(90) = 0.76068985340228 + 0.85787362659518i
x(91) = 0.76068985340228 + 0.85787362659518i
x(92) = 0.76068985340228 + 0.85787362659518i
x(93) = 0.76068985340228 + 0.85787362659518i
x(94) = 0.76068985340228 + 0.85787362659518i
x(95) = 0.76068985340228 + 0.85787362659518i

Muller's method

- Muller's method works for all types of functions, but more appropriate for the roots of the polynomials, since it has the ability to jump from real iterates to complex iterates and eventually can converge to a complex root.
- Choose $x_0,\ x_1,\ x_2$ so that $|f(x_0)| > |f(x_1)| > |f(x_2)|$. (Why?)
- What if $f(x_0) = f(x_1) = f(x_2)$?
- What if $(x_0, f(x_0)), (x_1, f(x_1)), (x_2, f(x_2))$ lie on a straight line?

Muller's method

- Next iterate x_3 with $sign(b)$ in the denominator is chosen ($x_3 = x_2 + \frac{-2c}{b \pm \sqrt{b^2 - 4ac}}$) so that the denominator will be the largest in magnitude and will result in choosing the root of $P(x)$ which is closest to x_2.
- The method is less sensitive to initial guesses when compared with Newton's and Secant methods.
- Order of convergence: Newton's method: $p = 2$; Secant method: $p \approx 1.618$; Muller's method: $p \approx 1.839$
- Muller's method avoids derivative calculation at every iteration.

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Thank You