Linear and Quadratic Order of convergence

DEFINITION Suppose $\{p_n\}_{n=1}^{\infty}$ is a sequence that converges to p with $p_n \neq p$ for all n. If positive constants λ and α exist with

$$\lim_{n \to \infty} \frac{|p_{n+1} - p|}{|p_n - p|^{\alpha}} = \lambda,$$

then $\{p_n\}_{n=1}^{\infty}$ converges to p of order α, with asymptotic error constant λ.

- If $\alpha = 2$, then $\{p_n\}_{n=1}^{\infty}$ converges quadratically.
- If $\alpha = 1$ and $\lambda < 1$, $\{p_n\}_{n=1}^{\infty}$ converges linearly.
- If $\alpha = 1$ and $\lambda = 0$, $\{p_n\}_{n=1}^{\infty}$ converges super-linearly.

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$\boxed{\alpha \geq 3 \text{ or higher does not typically work better than quadratic}}$

Recall and contrast: rate of convergence, the Big O

Suppose $\{\beta_n\}_{n=1}^{\infty}$ is a sequence known to converge to zero, and $\{\alpha_n\}_{n=1}^{\infty}$ converges to a number α. If a positive constant K exists with

$$|\alpha_n - \alpha| \le K|\beta_n|, \quad \text{for large } n,$$

then we say that $\{\alpha_n\}_{n=1}^{\infty}$ converges to α with **rate, or order, of convergence** $O(\beta_n)$. (This expression is read "big oh of β_n".) It is indicated by writing $\alpha_n = \alpha + O(\beta_n)$. ■

the Big $O()$ = rate of convergence

Linear and Quadratic Order of convergence (I)

- Suppose that $\{p_n\}_{n=1}^{\infty}$ is linearly convergent to 0,

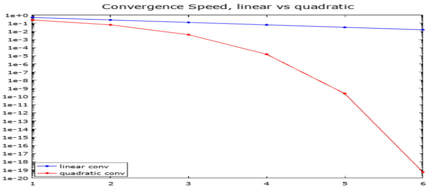
$$\lim_{n\to\infty} \frac{|p_{n+1}|}{|p_n|} = 0.5, \quad \text{or roughly} \quad \frac{|p_{n+1}|}{|p_n|} \approx 0.5,$$

hence $\boxed{p_n \approx (0.5)^n |p_0|.}$

- Suppose that $\{\tilde{p}_n\}_{n=1}^{\infty}$ is quadratically convergent to 0,

$$\lim_{n\to\infty} \frac{|\tilde{p}_{n+1}|}{|\tilde{p}_n|^2} = 0.5, \quad \text{or roughly} \quad \frac{|\tilde{p}_{n+1}|}{|\tilde{p}_n|^2} \approx 0.5.$$

$$\begin{aligned} \text{But} \quad 0.5\,|\tilde{p}_{n+1}| &\approx (0.5\,|\tilde{p}_n|)^2 \approx (0.5\,|\tilde{p}_{n-1}|)^{2^2} \approx \cdots \approx (0.5\,|\tilde{p}_1|)^{2^n} \\ |\tilde{p}_{n+1}| &\approx 2\,(0.5\,|\tilde{p}_1|)^{2^n} \end{aligned}$$



Order of convergence: Fixed Point Iteration (I)

Given initial approximation p_0, *Fixed Point Iteration* (FPI) is

$$p_n = g(p_{n-1}), \quad n = 1, 2, \cdots ,$$

Assume that

- FPI converges to fixed point p.
- $g(x)$ is continuously differentiable with $0 < |g'(p)| < 1$.

Theorem: FPI converges linearly,

$$\lim_{n\to\infty} \frac{|p_{n+1} - p|}{|p_n - p|} = |g'(p)|. \qquad (1)$$

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PROOF:

$$p_{n+1} - p \;=\; g(p_n) - g(p) = g'(\xi_n)\,(p_n - p),$$

where ξ_n is between p_n and p, and therefore converges to p.
(1) follows immediately.

Theorem 2.4 **(Fixed-Point Theorem)**

Let $g \in C[a,b]$ be such that $g(x) \in [a,b]$, for all x in $[a,b]$. Suppose, in addition, that g' exists on (a,b) and that a constant $0 < k < 1$ exists with

$$|g'(x)| \leq k, \quad \text{for all } x \in (a,b).$$

Then for any number p_0 in $[a,b]$, the sequence defined by

$$p_n = g(p_{n-1}), \quad n \geq 1,$$

converges to the unique fixed point p in $[a,b]$. ■

In FPI, $\quad |p_n - p| \leq k|p_{n-1} - p| \leq k^2|p_{n-2} - p| \leq \cdots \leq k^n|p_0 - p|.$

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recall Bisection convergence

Theorem 2.1 Suppose that $f \in C[a,b]$ and $f(a) \cdot f(b) < 0$. The Bisection method generates a sequence $\{p_n\}_{n=1}^{\infty}$ approximating a zero p of f with

$$|p_n - p| \leq \frac{b-a}{2^n}, \quad \text{when} \quad n \geq 1.$$ ■

Bisection Method is "considered" linearly convergent.

(Review) Newton's Method as Fixed Point Iteration

Assume $f(p) = 0$. Newton $=$ fixed point iteration

$$p_{k+1} = g(p_k), \quad k = 0, 1, \cdots, \qquad \text{where } g(x) = x - \frac{f(x)}{f'(x)}$$

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PROOF: By second order Taylor expansion,

$$g(p_n) \;=\; g(p) + g'(p)\,(p_n - p) + \frac{1}{2}\,g''(\xi_n)\,(p_n - p)^2,$$

where ξ_n is between p_n and p, and converges to p. So

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(1) follows immediately. $\boxed{\text{Newton's method satisfies } g'(p) = 0.}$

Order of convergence: Newton Method (again)

Given initial approximation p_0, *Newton Method* is

$$p_{n+1} = p_n - \frac{f(p_n)}{f'(p_n)}, \quad n = 0, 1, 2, \cdots ,$$

Assume that

- Newton Method converges to root p.
- $f''(x)$ is continuous with $f'(p) \neq 0$.

Theorem: Newton Method converges at least quadratically,

$$\lim_{n\to\infty} \frac{|p_{n+1} - p|}{|p_n - p|^2} = \frac{|f''(p)|}{2\,|f'(p)|}. \qquad (2)$$

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$$f(p) = f(p_n) + f'(p_n)\,(p - p_n) + \frac{1}{2}\, f''(\xi_n)\,(p - p_n)^2,$$

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$$p_{n+1} - p = p_n - p - \frac{f(p_n)}{f'(p_n)} = \frac{(p_n - p)\, f'(p_n) - f(p_n)}{f'(p_n)} = \frac{f''(\xi_n)}{2\, f'(p_n)}\,(p - p_n)^2,$$

and therefore (2) follows immediately.

Order of convergence: Secant Method (I)

Given initial approximations p_0, p_1, *Secant Method* is

$$p_{n+1} = p_n - \frac{f(p_n)(p_n - p_{n-1})}{f(p_n) - f(p_{n-1})}, n = 1, 2, \cdots .$$

Assume that

- Secant Method converges to root p.
- $f''(x)$ is continuous with $f'(p) \neq 0$.

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$$p_{n+1} = p_n - \frac{f(p_n)(p_n - p_{n-1})}{f(p_n) - f(p_{n-1})}, n = 1, 2, \cdots .$$

Assume that

- Secant Method converges to root p.
- $f''(x)$ is continuous with $f'(p) \neq 0$.

By Secant Method,

$$\begin{aligned}
p_{n+1} - p &= p_n - p - \frac{f(p_n)(p_n - p_{n-1})}{f(p_n) - f(p_{n-1})} \\
&= \frac{(p_n - p)\left(f(p_n) - f(p_{n-1})\right) - f(p_n)(p_n - p_{n-1})}{f(p_n) - f(p_{n-1})} \\
&= \frac{F(p_n) - F(p_{n-1})}{f(p_n) - f(p_{n-1})}\,(p_n - p)\,(p_{n-1} - p),
\end{aligned}$$

where $F(x) \overset{def}{=} \frac{f(x) - f(p)}{x - p}$ is differentiable with $F(p) \overset{def}{=} f'(p)$.

Order of convergence: Secant Method (II)

Assume that

- Secant Method converges to root p.
- $f''(x)$ is continuous with $f'(p) \neq 0$.

Theorem: Secant Method converges at order $\alpha = \frac{1+\sqrt{5}}{2}$,

$$\lim_{n\to\infty} \frac{|p_{n+1} - p|}{|p_n - p|^\alpha} = \texttt{constant}. \qquad (3)$$

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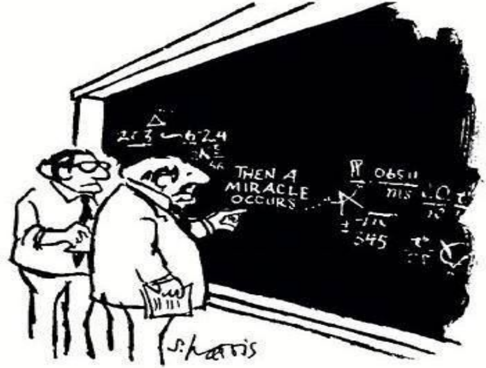
PROOF: With $F(x) \stackrel{def}{=} \frac{f(x)-f(p)}{x-p}$,

$$p_{n+1} - p = \frac{F(p_n) - F(p_{n-1})}{f(p_n) - f(p_{n-1})} (p_n - p)(p_{n-1} - p),$$

we can show that ratio converges to $\frac{f''(p)}{2 f'(p)}$ and that α satisfies $\alpha(\alpha - 1) = 1$, therefore

$$\frac{|p_{n+1} - p|}{|p_n - p|^\alpha} = \left|\frac{F(p_n) - F(p_{n-1})}{f(p_n) - f(p_{n-1})}\right| \left(\frac{|p_n - p|}{|p_{n-1} - p|^\alpha}\right)^{-(\alpha-1)}$$

$$\frac{|p_{n+1}-p|}{|p_n-p|^\alpha} = \left|\frac{F(p_n)-F(p_{n-1})}{f(p_n)-f(p_{n-1})}\right| \left(\frac{|p_n-p|}{|p_{n-1}-p|^\alpha}\right)^{-(\alpha-1)}$$

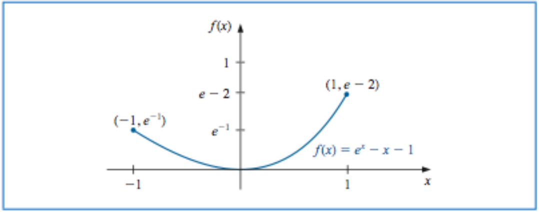


"I THINK YOU SHOULD BE MORE EXPLICIT HERE IN STEP TWO."

CLAIM: $\lim_{n\to\infty} \frac{|p_{n+1}-p|}{|p_n-p|^\alpha}$ exists $\implies$ $\lim_{n\to\infty} \frac{|p_{n+1}-p|}{|p_n-p|^\alpha} = \left|\frac{f''(p)}{2\,f'(p)}\right|^{\frac{1}{\alpha}}$

Example I: $f(x) = e^x - x - 1$, $f(0) = f'(0) = 0$, $f''(0) = 1$

Function



Newton's Method

n	p_n
0	1.0
1	0.58198
2	0.31906
3	0.16800
4	0.08635
5	0.04380
6	0.02206
7	0.01107
8	0.005545
9	2.7750×10^{-3}
10	1.3881×10^{-3}
11	6.9411×10^{-4}
12	3.4703×10^{-4}
13	1.7416×10^{-4}
14	8.8041×10^{-5}
15	4.2610×10^{-5}
16	1.9142×10^{-6}

Much worse than typical Newton method convergence behavior

Simple root: $f(p) = 0, f'(p) \neq 0$

- **Definition**: A solution p of $f(x) = 0$ is a *simple root* if $f(p) = 0$ and $f'(p) \neq 0$.
- **Theorem**: The function $f \in C^1[a, b]$ has a simple root at p in (a, b) if and only if

$$f(x) = (x - p)\, q(x), \quad \text{where} \quad \lim_{x \to p} q(x) \neq 0.$$

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PROOF of "only if": Assume $f(p) = 0$ and $f'(p) \neq 0$. Define for $x \neq p$,

$$q(x) = \frac{f(x) - f(p)}{x - p} = \frac{f(x)}{x - p},$$

$$\text{then} \quad \lim_{x \to p} q(x) = \lim_{x \to p} \frac{f(x) - f(p)}{x - p} = f'(p) \neq 0.$$

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PROOF of "if": Assume $f(x) = (x - p)\, q(x)$. Then $f(p) = 0$ and

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Multiple roots: $f(p) = 0, f'(p) = 0$

- **Definition**: A solution p of $f(x) = 0$ is a root of multiplicity m (with integer m) of f if for $x \neq p$, we can write

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- **Theorem**: The function $f \in C^m[a, b]$ has a root of multiplicity m at p in (a, b) if and only if

$$0 = f(p) = f'(p) = f''(p) = \cdots = f^{(m-1)}(p), \ \text{ but } \ f^{(m)}(p) \neq 0.$$

- **simple root** $(m = 1)$: f satisfies $f(p) = 0$, but $f'(p) \neq 0$.

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(Recall) Quadratic Convergence for Newton Method

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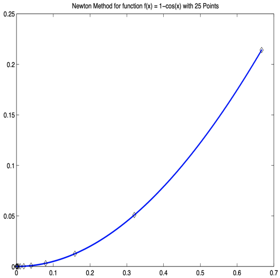
$$\boxed{\text{Right hand side in (1) not defined if } f'(p) = 0.}$$

Example II: $f(x) = 1 - \cos x, f(0) = f'(0) = 0, f''(0) = 1$ Number of iterations vs. Magnitude in function values



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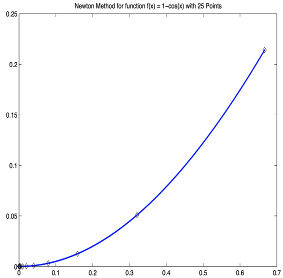

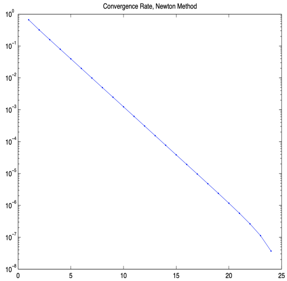

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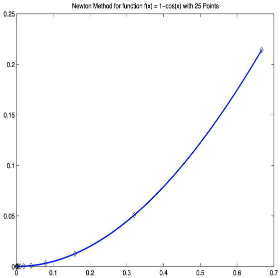
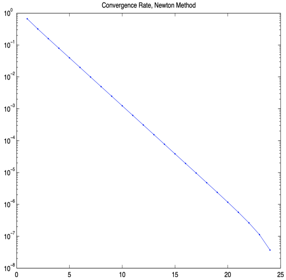


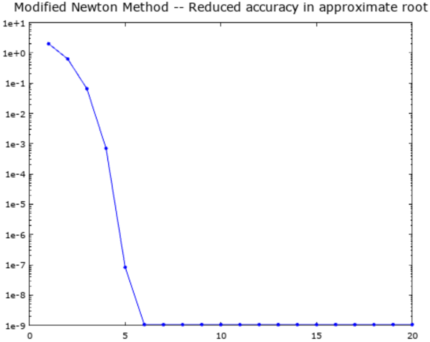


If $|x| \le 10^{-8}$, then $|f(x)| = 1 - \cos x = 2\sin^2 \frac{x}{2} \le 10^{-16}$.

Modified Newton Method

$$p_{k+1} = p_k - \frac{m\, f(p_k)}{f'(p_k)}, \quad \text{for} \quad k = 1, 2, \cdots, \quad \text{(must know multiplicity } m \text{ of root)}$$

- $m = 2$ for function $f(x) = e^x - x - 1$,



- $|f(p_k)|$ drops to $O(10^{-9})$ only, far from machine precision $O(10^{-16})$.

Modified Newton Method is Quadratically Convergent

$$p_{k+1} = g(p_k), \quad g(x) = x - \frac{m\, f(x)}{f'(x)}, \text{ for } k = 1, 2, \cdots,$$

PROOF of quadratic convergence:

- Let $f(x) = (x-p)^m q(x), \quad q(p) \neq 0.$
- Write $g(x)$ in terms of $q(x)$:

$$g(x) = x - \frac{m\, f(x)}{f'(x)} = x - \frac{m\,(x-p)q(x)}{mq(x) + (x-p)q'(x)}.$$

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- Terms cancel in $g'(x)$:

$$\begin{aligned} g'(x) &= 1 - \frac{m\, q(x)}{mq(x) + (x-p)q'(x)} - m\,(x-p)\left(\frac{q(x)}{mq(x) + (x-p)q'(x)}\right)' \\ &= \frac{(x-p)q'(x)}{mq(x) + (x-p)q'(x)} - m(x-p)\left(\frac{q(x)}{mq(x) + (x-p)q'(x)}\right)' \end{aligned}$$

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- $g'(p) = 0$, hence quadratic convergence
  (by fixed point iteration convergence theorem.)

Modified Newton Method in textbook

$$p_{k+1} = g(p_k), \quad g(x) = x - \frac{f(x)\, f'(x)}{\left(f'(x)\right)^2 - f(x)\, f''(x)}, \text{ for } k = 1, 2, \cdots,$$

- Also quadratic convergence.
- Even less practical since second order derivative is involved.

§2.5 Accelerating Convergence: Aitken's Δ^2 Method

- **Suppose** $\{p_k\}_{k=1}^{\infty}$ linearly converges to limit p,

$$\lim_{k\to\infty} \frac{p_{k+1}-p}{p_k-p} = \lambda, \quad |\lambda| < 1.$$

- **Define**

$$\frac{p_{k+1}-p}{p_k-p} \stackrel{def}{=} \lambda_k,$$

  so that $\{\lambda_k\}_{k=1}^{\infty}$ converges to λ.

- It follows that

$$0 \approx \lambda_{k+1} - \lambda_k = \frac{p_{k+2}-p}{p_{k+1}-p} - \frac{p_{k+1}-p}{p_k-p}.$$

- Solve for p:

$$p = \frac{p_{k+1}^2 - p_k p_{k+2}}{2p_{k+1} - p_k - p_{k+2}} + \frac{(\lambda_{k+1}-\lambda_k)(p_{k+1}-p)(p_k-p)}{2(p_{k+1}-p)-(p_k-p)-(p_{k+2}-p)}.$$

Accelerating Convergence: Aitken's Δ^2 Method

$$\begin{aligned}
\widehat{p}_k &\stackrel{def}{=} \frac{p_{k+1}^2 - p_k p_{k+2}}{2p_{k+1} - p_k - p_{k+2}} \\
&= p_k - \frac{(p_{k+1} - p_k)^2}{p_{k+2} - 2p_{k+1} + p_k} \stackrel{def}{=} \{\Delta^2\}(p_k).
\end{aligned}$$

Approximation Error

$$\begin{aligned}
|\widehat{p}_k - p| &= \left| \frac{(\lambda_{k+1} - \lambda_k)(p_{k+1} - p)(p_k - p)}{2(p_{k+1} - p) - (p_k - p) - (p_{k+2} - p)} \right| \\
&= \left| \frac{(\lambda_{k+1} - \lambda_k)(p_k - p)}{2 - \left(\frac{p_{k+1} - p}{p_k - p}\right)^{-1} - \frac{p_{k+2} - p}{p_{k+1} - p}} \right| \\
&\approx \left| \frac{(\lambda_{k+1} - \lambda_k)(p_k - p)}{2 - \lambda^{-1} - \lambda} \right| \ll O\left(|p_k - p|\right),
\end{aligned}$$

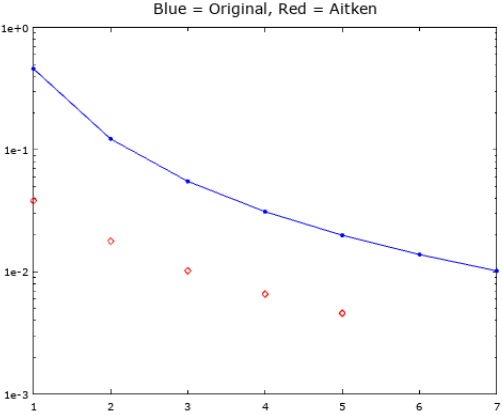
since $\lambda_{k+1} - \lambda_k \approx 0$.

Accelerating Convergence: Aitken's Δ^2 Method

$p_n = \cos(1/n)$

n	p_n	$\hat{p}_n$
1	0.54030	0.96178
2	0.87758	0.98213
3	0.94496	0.98979
4	0.96891	0.99342
5	0.98007	0.99541
6	0.98614	
7	0.98981	

Error: $|p_n - 1|$ vs $|\widehat{p}_n - 1|$



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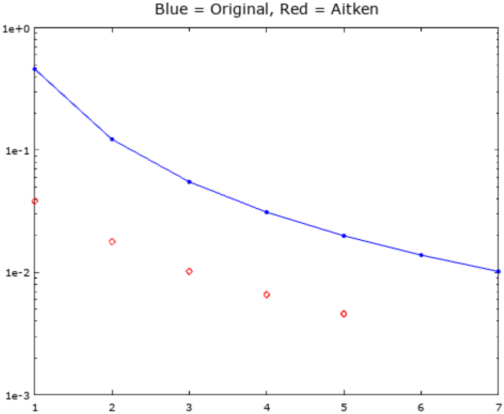
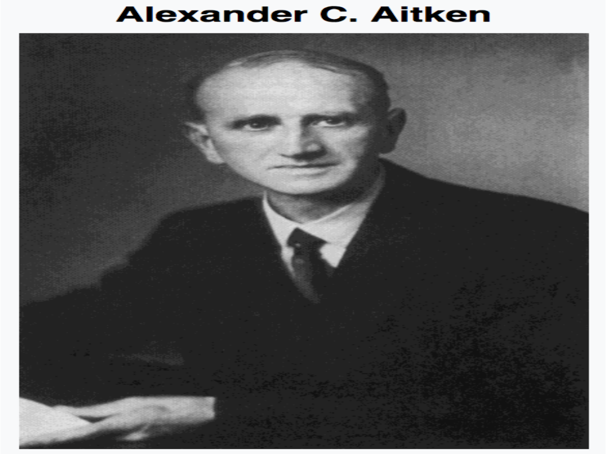


Error decays more quickly, but not quick enough.



- Big data scientist well before big data. Ph.D. thesis (1925) *Smoothing of Data*.
- Remembered the first 1000 digits of π.

Accelerating Convergence: Steffensen's Method (I)

- (Recall) fixed point iteration (FPI)

$$p_{k+1} = q(p_k), \quad k = 0, 1, \cdots \qquad (1)$$

Accelerating Convergence: Steffensen's Method (I)

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- (Recall) Aitken's Acceleration for a given $\{p_k\}_{k=1}^{\infty}$:

$$\{\Delta^2\}(p_k) = p_k - \frac{(p_{k+1} - p_k)^2}{p_{k+2} - 2p_{k+1} + p_k}. \tag{2}$$

Accelerating Convergence: Steffensen's Method (I)

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Steffensen's Dilemma

- Aitken (2) can accelerate FPI (1)

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- (Recall) fixed point iteration (FPI)

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$$\{\Delta^2\}(p_k) = p_k - \frac{(p_{k+1} - p_k)^2}{p_{k+2} - 2p_{k+1} + p_k}. \qquad (2)$$

Steffensen's Dilemma

- Aitken (2) can accelerate FPI (1)

- Won't need Aitken (2) given $\{p_k\}$ from (1)

Accelerating Convergence: Steffensen's Method (II)

- Given $p_0^{(0)}$, do two fixed point iterations:

$$p_1^{(0)} = g(p_0^{(0)}), \;\; p_2^{(0)} = g(p_1^{(0)}).$$

- Let Aitken compute a better approximation:

$$p_0^{(1)} = \{\Delta^2\}(p_0^{(0)}),$$

  $p_0^{(1)}$ also comes for "free" since it does not involve g function.

- Resume with two fixed point iterations on $p_0^{(1)}$.

$$p_1^{(1)} = g(p_0^{(1)}), \;\; p_2^{(1)} = g(p_1^{(1)}).$$

- Again let Aitken compute a better approximation:

$$p_0^{(2)} = \{\Delta^2\}(p_0^{(1)}).$$

- Repeat with two fixed point iterations on $p_0^{(2)}$.

Accelerating Convergence: Steffensen's Method (III)

- Steffensen's Method: use one Aitken's Acceleration after every two fixed point iterations:
  - Given $p_0^{(0)}$, repeat:

$$p_1^{(0)} = g(p_0^{(0)}), \;\; p_2^{(0)} = g(p_1^{(k)}), \;\; p_0^{(1)} = \{\Delta^2\}(p_0^{(0)})$$

Accelerating Convergence: Steffensen's Method (III)

- Steffensen's Method: use one Aitken's Acceleration after every two fixed point iterations:
  - Given $p_0^{(0)}$, repeat:

$$
\begin{aligned}
p_1^{(0)} &= g(p_0^{(0)}), \;\; p_2^{(0)} = g(p_1^{(k)}), \;\; p_0^{(1)} = \{\Delta^2\}(p_0^{(0)}) \\
p_1^{(1)} &= g(p_0^{(1)}), \;\; p_2^{(1)} = g(p_1^{(1)}), \;\; p_0^{(2)} = \{\Delta^2\}(p_0^{(1)})
\end{aligned}
$$

Accelerating Convergence: Steffensen's Method (III)

- Steffensen's Method: use one Aitken's Acceleration after every two fixed point iterations:
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\begin{array}{rcl}
p_1^{(0)} & = & g(p_0^{(0)}), \;\; p_2^{(0)} = g(p_1^{(k)}), \;\; p_0^{(1)} = \{\Delta^2\}(p_0^{(0)}) \\
p_1^{(1)} & = & g(p_0^{(1)}), \;\; p_2^{(1)} = g(p_1^{(1)}), \;\; p_0^{(2)} = \{\Delta^2\}(p_0^{(1)}) \\
\vdots & = & \vdots \\
p_1^{(k)} & = & g(p_0^{(k)}), \;\; p_2^{(k)} = g(p_1^{(k)}), \;\; p_0^{(k+1)} = \{\Delta^2\}(p_0^{(k)})
\end{array}
$$

- Method converges when $\left|p_0^{(k+1)} - p_0^{(k)}\right| < \texttt{tolerance}$

Steffensen's

To find a solution to $p = g(p)$ given an initial approximation p_0:

INPUT initial approximation p_0; tolerance TOL; maximum number of iterations N_0.

OUTPUT approximate solution p or message of failure.

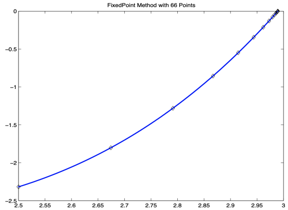
Step 1 Set $i = 1$.

Step 2 While $i \leq N_0$ do Steps 3–6.

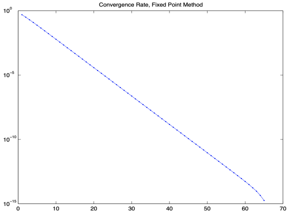
> ***Step 3*** Set $p_1 = g(p_0)$; (*Compute* $p_1^{(i-1)}$.)
> $p_2 = g(p_1)$; (*Compute* $p_2^{(i-1)}$.)
> $p = p_0 - (p_1 - p_0)^2/(p_2 - 2p_1 + p_0)$. (*Compute* $p_0^{(i)}$.)
>
> ***Step 4*** If $|p - p_0| < TOL$ then
> OUTPUT (p); (*Procedure completed successfully.*)
> STOP.
>
> ***Step 5*** Set $i = i + 1$.
>
> ***Step 6*** Set $p_0 = p$. (*Update* p_0.)

Step 7 OUTPUT ('Method failed after N_0 iterations, N_0 =', N_0);
(*Procedure completed unsuccessfully.*)
STOP.

- Fixed point for $g(x) = log(2 + 2x^2)$



- FPI Linear Convergence



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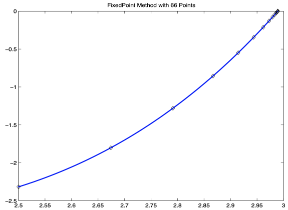

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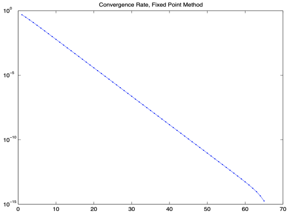
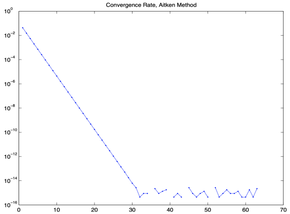
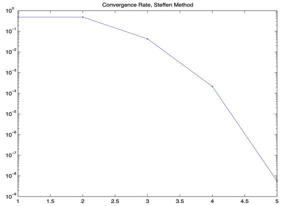


- Aitken's Method on FPI



- Steffenson: Quadratic Convergence



Order of Convergence: Steffenson's Method

Given initial approximation p_0, $\boxed{\text{convergent FPI map}}$ $g(x)$ with $\boxed{g'(p) \neq 1}$, *Steffenson's Method* is

$$p_n = G(p_{n-1}), \quad n = 1, 2, \cdots, \quad G(x) = x - \frac{(g(x) - x)^2}{g(g(x)) - 2\,g(x) + x}.$$

Assume

- Steffenson's Method converges to fixed point p.
- $g''(x)$ is continuously differentiable, and $g'(p) - 1 \neq 0$.

Theorem: Steffenson's Method converges at least quadratically.

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PROOF:

$$\begin{aligned} G'(x) &= 1 - \left(g'(x) - 1\right) \cdot \left(\frac{g(x) - x}{g(g(x)) - 2\,g(x) + x}\right) \\ &\quad - \left(g(x) - x\right) \cdot \left(\frac{g(x) - x}{g(g(x)) - 2\,g(x) + x}\right)' \\ G'(p) &= 1 - \left(g'(p) - 1\right) \cdot \frac{\left(g(x) - x\right)'_{x=p}}{\left(g(g(x)) - 2\,g(x) + x\right)'_{x=p}} \end{aligned}$$

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Proof:
$$\begin{aligned} G'(x) &= 1 - \left(g'(x) - 1\right) \cdot \left(\frac{g(x) - x}{g(g(x)) - 2\,g(x) + x}\right) \\ &\quad - \left(g(x) - x\right) \cdot \left(\frac{g(x) - x}{g(g(x)) - 2\,g(x) + x}\right)' \\ G'(p) &= 1 - \left(g'(p) - 1\right) \cdot \frac{\left(g(x) - x\right)'_{x=p}}{\left(g(g(x)) - 2\,g(x) + x\right)'_{x=p}} \end{aligned}$$

Hence $G'(p) = 0$, implying quadratic convergence.

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Hence $G'(p) = 0$, implying quadratic convergence.

$\boxed{\text{What would be a good } g(x)?}$

Steffenson + Newton on multiple root = quadratically convergent

Given initial approximation p_0, $\boxed{\text{convergent FPI map}}$ $g(x)$ with $\boxed{g'(p) \neq 1}$, *Steffenson's Method* is

$$p_n = G(p_{n-1}), \quad n = 1, 2, \cdots, \quad G(x) = x - \frac{(g(x) - x)^2}{g(g(x)) - 2\,g(x) + x}$$

Choose $\quad g(x) = x - \dfrac{f(x)}{f'(x)},\;$ for $\; f(x) = (x-p)^m\, q(x), \;\; q(p) \neq 0$

Proof of quadratic convergence:

- Write $g(x)$ in terms of $q(x)$:

$$g(x) = x - \frac{f(x)}{f'(x)} = x - \frac{(x-p)q(x)}{mq(x) + (x-p)q'(x)}.$$

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Given initial approximation p_0, $\boxed{\text{convergent FPI map}}$ $g(x)$ with $\boxed{g'(p) \neq 1}$, *Steffenson's Method* is

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Choose $\quad g(x) = x - \dfrac{f(x)}{f'(x)}, \quad$ for $\; f(x) = (x-p)^m\; q(x), \quad q(p) \neq 0$

Proof of quadratic convergence:

- Write $g(x)$ in terms of $q(x)$:

$$g(x) = x - \frac{f(x)}{f'(x)} = x - \frac{(x-p)q(x)}{mq(x) + (x-p)q'(x)}.$$

$$\begin{aligned} g'(x) &= 1 - \frac{q(x)}{mq(x) + (x-p)q'(x)} - (x-p)\left(\frac{q(x)}{mq(x) + (x-p)q'(x)}\right)' \\ g'(p) &= 1 - \frac{1}{m} \neq 1 \end{aligned}$$

(Review) Horner's Method for nested arithmetic

Evaluate function $P(x)$ for given x:

$$\begin{aligned} P(x) &= a_0 + a_1 x + \cdots + a_n x^n \\ &= a_0 + x \cdot (a_1 + x \cdot (\cdots + x \cdot (a_{n-1} + x \cdot a_n) \cdots)) \end{aligned}$$

§2.6 Newton's Method on Polynomials (Horner's Method)

$$\text{Let} \quad P(x) = a_0 + a_1 x + \cdots + a_n x^n$$
$$= a_0 + x \cdot (a_1 + x \cdot (\cdots + x \cdot (a_{n-1} + x \cdot a_n) \cdots))$$

Horner's Method computes $P(x_0)$

- **define** $b_n = a_n$
- **for** $k = n-1, n-2, \cdots, 1, 0$

$$b_k = a_k + b_{k+1} x_0, \qquad (1)$$

- then $b_0 = P(x_0)$.

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$$b_k = a_k + b_{k+1} x_0, \qquad (1)$$

- then $b_0 = P(x_0)$.

Theorem: Horner's Method further computes

$$P(x) = (x - x_0)\, Q(x) + b_0, \text{ with } Q(x) = b_n x^{n-1} + b_{n-1} x^{n-2} + \cdots + b_2 x + b_1.$$

Newton's Method on Polynomials (Horner's Method) (II)

- **define** $b_n = a_n$
- **for** $k = n-1, n-2, \cdots, 1, 0$

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PROOF: From (1), $b_k - b_{k+1} x_0 = a_k$, for $k = n-1, \cdots, 0$.

$$\begin{aligned}
(x - x_0)\, Q(x) + b_0 &= b_n\, x^n + b_{n-1}\, x^{n-1} + \cdots + b_2\, x^2 + b_1\, x + b_0 \\
&\quad - \left(x_0\, b_n\, x^{n-1} + x_0\, b_{n-1} x^{n-2} + \cdots + x_0\, b_2\, x + x_0\, b_1\right) \\
&= b_n\, x^n + (b_{n-1} - x_0\, b_n)\, x^{n-1} + \cdots + (b_0 - x_0\, b_1) \\
&= P(x)
\end{aligned}$$

Newton's Method on Polynomials (Horner's Method) (III)

- **define** $b_n = a_n$
- **for** $k = n-1, n-2, \cdots, 1, \boxed{0}$

$$b_k = a_k + b_{k+1} x_0, \qquad (1)$$

Theorem: Horner's Method further computes

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$$b_k = a_k + b_{k+1} x_0, \qquad (1)$$

Theorem: Horner's Method further computes

$$P(x) = (x - x_0)\, Q(x) + b_0, \text{ with } Q(x) = b_n\, x^{n-1} + b_{n-1} x^{n-2} + \cdots + b_2 x + b_1.$$

Since $\quad P'(x) = Q(x) + (x - x_0)\, Q'(x), \quad$ we have $\quad P'(x_0) = Q(x_0).$

Single **for** loop for $P(x_0)$ and $Q(x_0) = P'(x_0)$ (Newton Method):

- **define** $c_n = b_n = a_n$
- **for** $k = n-1, n-2, \cdots, \boxed{1}$

$$b_k \;=\; a_k + b_{k+1} x_0, \qquad c_k = b_k + c_{k+1} x_0,$$

- $Q(x_0) = c_1$ and $P(x_0) = a_0 + b_1 x_0$.

Horner's Method

INPUT degree n; coefficients $a_0, a_1, \ldots, a_n$; x_0.

OUTPUT $y = P(x_0)$; $z = P'(x_0)$.

Step 1 Set $y = a_n$; (*Compute b_n for P.*)
$z = a_n$. (*Compute b_{n-1} for Q.*)

Step 2 For $j = n-1, n-2, \ldots, 1$
set $y = x_0 y + a_j$; (*Compute b_j for P.*)
$z = x_0 z + y$. (*Compute b_{j-1} for Q.*)

Step 3 Set $y = x_0 y + a_0$. (*Compute b_0 for P.*)

Step 4 OUTPUT (y, z);
STOP.

Deflation Procedure for finding all roots of a Polynomial

1. Given polynomial $P(x)$ of degree n

$$P(x) = a_n\, x^n + b_{n-1}\, x^{n-1} + \cdots + a_2\, x^2 + a_1\, x + a_0 \quad \text{with} \quad a_n \neq 0.$$

Would like to find <u>all</u> n roots in $P(x) = 0$.

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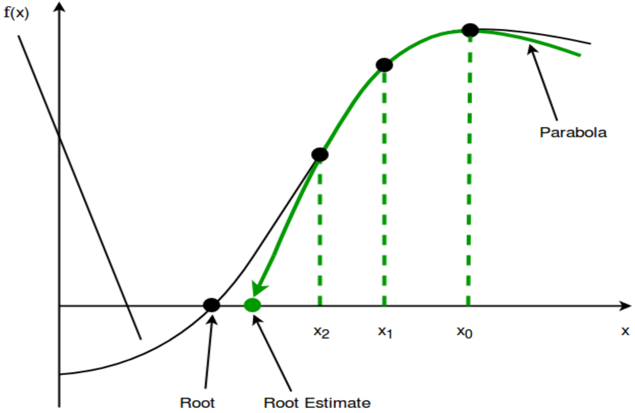
4. Find all other $n - 1$ roots in $P(x) = 0$ by recursively solving

$$Q(x) = 0.$$

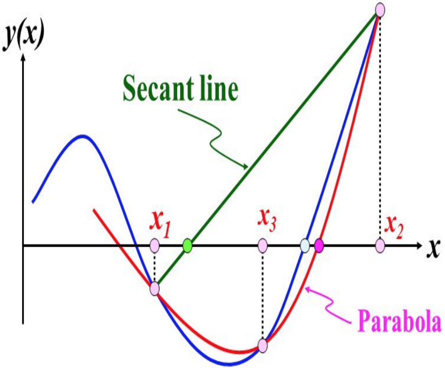
$\boxed{\text{CATCH: Do not yet know how to compute complex roots}}$

Muller's Method: finding complex roots

- **Given** three points $(p_0, f(p_0)), (p_1, f(p_1))$, and $(p_2, f(p_2))$.
- **Construct** a parabola through them,
- p_3 is the intersection with x-axis <u>closest</u> to p_2.



Secant Method vs. Muller's Method



- Secant Method requires two points $(p_0, f(p_0)), (p_1, f(p_1))$, with <u>one</u> x-axis intercept in green.
- Muller's Method requires three points $(p_0, f(p_0)), (p_1, f(p_1))$, and $(p_2, f(p_2))$, with <u>two</u> REAL (or COMPLEX) x-axis intercepts in red.

Muller's Method: derivation

1. Choose parabola $P(x) = a\,(x - p_2)^2 + b\,(x - p_2) + c,$

where a, b, c satisfy
$$\begin{aligned} f(p_0) &= a\,(p_0 - p_2)^2 + b\,(p_0 - p_2) + c, \\ f(p_1) &= a\,(p_1 - p_2)^2 + b\,(p_1 - p_2) + c, \\ f(p_2) &= c. \end{aligned}$$

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2. So $c = f(p_2)$, and

$$\begin{aligned} \frac{f(p_0) - f(p_2)}{p_0 - p_2} &= a\,(p_0 - p_2) + b, \\ \frac{f(p_1) - f(p_2)}{p_1 - p_2} &= a\,(p_1 - p_2) + b. \end{aligned}$$

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$$
\begin{aligned}
f(p_0) &= a\,(p_0 - p_2)^2 + b\,(p_0 - p_2) + c,\\
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f(p_2) &= c.
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\begin{aligned}
\frac{f(p_0) - f(p_2)}{p_0 - p_2} &= a\,(p_0 - p_2) + b,\\
\frac{f(p_1) - f(p_2)}{p_1 - p_2} &= a\,(p_1 - p_2) + b.
\end{aligned}
$$

3. Therefore
$$
\begin{aligned}
a &= \frac{1}{p_0 - p_1}\left(\frac{f(p_0) - f(p_2)}{p_0 - p_2} - \frac{f(p_1) - f(p_2)}{p_1 - p_2}\right),\\
b &= \frac{f(p_0) - f(p_2)}{p_0 - p_2} - a\,(p_0 - p_2).
\end{aligned}
$$

Muller's Method: finding p_3

1 Muller's parabola $\quad P(x) = a\,(x-p_2)^2 + b\,(x-p_2) + c,$

with roots of $P(x) = 0$ satisfy $\quad p_3 = p_2 + \dfrac{-b \pm \sqrt{b^2 - 4\,a\,c}}{2\,a}.$

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2 Choose sign in $\pm$ so p_3 is closest to p_2:

$$p_3 \quad = \quad p_2 + \frac{-b + \textbf{sign}\,(b)\,\sqrt{b^2 - 4\,a\,c}}{2\,a}$$

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2. Choose sign in $\pm$ so p_3 is closest to p_2:

$$
\begin{aligned}
p_3 &= p_2 + \frac{-b + \mathbf{sign}\,(b)\,\sqrt{b^2 - 4\,a\,c}}{2\,a} \\
&= p_2 + \frac{\left(-b + \mathbf{sign}\,(b)\,\sqrt{b^2 - 4\,a\,c}\right)\left(b + \mathbf{sign}\,(b)\,\sqrt{b^2 - 4\,a\,c}\right)}{2\,a\left(b + \mathbf{sign}\,(b)\,\sqrt{b^2 - 4\,a\,c}\right)} \\
&= p_2 - \frac{2\,c}{b + \mathbf{sign}\,(b)\,\sqrt{b^2 - 4\,a\,c}}, \quad (\textit{numerically more stable})
\end{aligned}
$$

Muller's Method: finding p_3

(1) Muller's parabola $P(x) = a\,(x - p_2)^2 + b\,(x - p_2) + c,$

with roots of $P(x) = 0$ satisfy $p_3 = p_2 + \dfrac{-b \pm \sqrt{b^2 - 4\,a\,c}}{2\,a}.$

(2) Choose sign in $\pm$ so p_3 is closest to p_2:

$$\begin{aligned}
p_3 &= p_2 + \frac{-b + \mathbf{sign}\,(b)\,\sqrt{b^2 - 4\,a\,c}}{2\,a} \\
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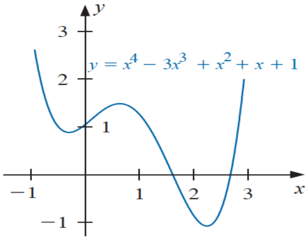
&= p_2 - \frac{2\,c}{b + \mathbf{sign}\,(b)\,\sqrt{b^2 - 4\,a\,c}}, \quad (\textit{numerically more stable})
\end{aligned}$$

(3) Notational convention

$$\mathbf{sign}\,(b) = \mathbf{sign}\,(\mathbf{real}\,(b))\,, \quad \mathbf{real}\left(\sqrt{b^2 - 4\,a\,c}\right) \geq 0.$$

Muller's Method: $p_0 = 0.5, p_1 = -0.5, p_2 = 0$, root $p \approx -0.339 + 0.447i$

- Function has real & complex roots.



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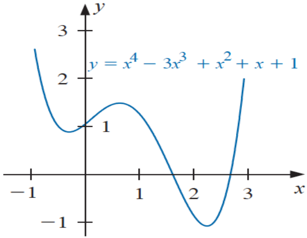
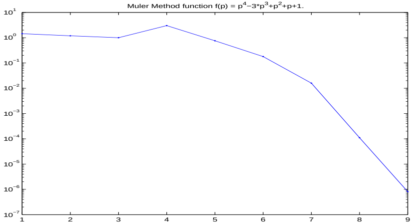


- Muller's method converges to complex root in 9 iterations.



Order of Convergence: Muller's Method (I)

Given three approximations $p_{n-2},\ p_{n-1}, p_n$, Muller's parabola

$$\begin{aligned} P(x) &= a\,(x-p_n)^2 + b\,(x-p_n) + c \quad \text{satisfies} \\ f(p_j) &= P(p_j), \quad j = n-2, n-1, n, \quad \text{and} \quad P(p_{n+1}) = 0. \end{aligned}$$

Assume that

- Muller's converges to root p.
- $f'''(x)$ is continuous with $f'(p) \neq 0$.

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f(p_j) &= P(p_j), \quad j = n-2, n-1, n, \quad \text{and} \quad P(p_{n+1}) = 0.
\end{aligned}
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Assume that

- Muller's converges to root p.
- $f'''(x)$ is continuous with $f'(p) \neq 0$.

1 By def, $F(x) \stackrel{def}{=} f(x) - P(x)$ must have roots at $x = p_{n-2}$, p_{n-1}, p_n. Therefore there is differentiable function $Q_1(x)$ so

$$f(x) - P(x) = F(x) = (x - p_{n-2})\,(x - p_{n-1})\,(x - p_n)\;Q_1(x).$$

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Given three approximations p_{n-2}, p_{n-1}, p_n, Muller's parabola

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2 Similarly $P(x) = (x - p_{n+1})\,Q_2(x)$ for some function $Q_2(x)$.

Order of Convergence: Muller's Method (I)

Given three approximations p_{n-2}, p_{n-1}, p_n, Muller's parabola

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1 By def, $F(x) \stackrel{def}{=} f(x) - P(x)$ must have roots at $x = p_{n-2}$, p_{n-1}, p_n. Therefore there is differentiable function $Q_1(x)$ so

$$f(x) - P(x) = F(x) = (x - p_{n-2})\,(x - p_{n-1})\,(x - p_n)\,Q_1(x).$$

2 Similarly $P(x) = (x - p_{n+1})\,Q_2(x)$ for some function $Q_2(x)$.

3 Together: $$\begin{aligned} p - p_{n+1} &= \frac{P(p)}{Q_2(p)} = -\frac{f(p) - P(p)}{Q_2(p)} \\ &= -\frac{Q_1(p)}{Q_2(p)}\,(p - p_{n-2})\,(p - p_{n-1})\,(p - p_n)\,, \end{aligned}$$

where ratio converges to $f'''(p)\,/\,(6\,f'(p))$.

Order of Convergence: Muller's Method (II)

Assume that

- Muller's Method converges to root p.
- $f'''(x)$ is continuous with $f'(p) \neq 0$.

Theorem: Muller's Method converges at order $\mu \approx 1.84$, with $\mu^3 = \mu^2 + \mu + 1$.

$$\lim_{n \to \infty} \frac{|p_{n+1} - p|}{|p_n - p|^{\mu}} = \texttt{constant}.$$

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- Muller's Method converges to root p.
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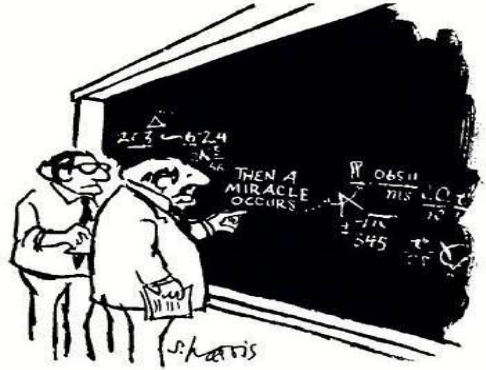
$$\lim_{n\to\infty} \frac{|p_{n+1} - p|}{|p_n - p|^\mu} = \texttt{constant}.$$

PROOF: $p_{n+1} - p = \dfrac{Q_1(p)}{Q_2(p)} \left(p - p_{n-2}\right)\left(p - p_{n-1}\right)\left(p - p_n\right),$

therefore $\dfrac{|p_{n+1} - p|}{|p_n - p|^\mu} = \left|\dfrac{Q_1(p)}{Q_2(p)}\right| \left(\dfrac{|p_n - p|}{|p_{n-1} - p|^\mu}\right)^{1-\mu} \left(\dfrac{|p_{n-1} - p|}{|p_{n-2} - p|^\mu}\right)^{1+\mu-\mu^2}.$

$$\frac{|p_{n+1}-p|}{|p_n-p|^{\mu}} = \left|\frac{Q_1(p)}{Q_2(p)}\right| \left(\frac{|p_n-p|}{|p_{n-1}-p|^{\mu}}\right)^{1-\mu} \left(\frac{|p_{n-1}-p|}{|p_{n-2}-p|^{\mu}}\right)^{1+\mu-\mu^2}.$$



"I THINK YOU SHOULD BE MORE EXPLICIT HERE IN STEP TWO."

CLAIM: $\displaystyle\lim_{n\to\infty} \frac{|p_{n+1}-p|}{|p_n-p|^{\mu}}$ exists. $\longrightarrow$ $\displaystyle\lim_{n\to\infty} \frac{|p_{n+1}-p|}{|p_n-p|^{\mu}} = \left|\frac{f'''(p)}{6\,f'(p)}\right|^{\frac{1}{\mu^2-1}}.$

Deflation Procedure for finding all roots of a Polynomial

1 Given polynomial $P(x)$ of degree n

$$P(x) = a_n\, x^n + b_{n-1}\, x^{n-1} + \cdots + a_2\, x^2 + a_1\, x + a_0 \quad \text{with} \quad a_n \neq 0.$$

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Would like to find <u>all</u> n roots in $P(x) = 0$.

2. Let Horner's Method compute

$$P(x) = (x - x_0)\, Q(x) + b_0, \text{ with } Q(x) = b_n\, x^{n-1} + b_{n-1}\, x^{n-2} + \cdots + b_2\, x + b_1,$$

after finding x_0 with a root-finder (*i.e.* Newton, bisection, or Muller.)

3. An approximate root $x \approx x_0$ of $P(x) = 0$ is found if

$$|b_0| \leq \texttt{tol} \quad \text{for tolerance} \quad \texttt{tol}. \quad (1) \quad \Longrightarrow P(x) \approx (x - x_0)\, Q(x)$$

4. Find all other $n-1$ roots in $P(x) = 0$ by recursively solving

$$Q(x) = 0.$$

$\boxed{\text{QUESTION: Can we find all polynomial roots now?}}$

Deflation: $f(x) = x^4 - 3\,x^3 + x^2 + x + 1$, root $p \approx -0.339093 + 0.446630i$

- root p is accurate to about 7 digits.

```
>>
>> aa = [1 -3 1 1 1];
>>
>> a = fliplr(aa);
>>
>> x = -0.339093+0.446630i;
>>
>> b = horner2(a,x); abs(b)
ans =

   8.1011e-07   1.7833e+00   2.5366e+00   3.3688e+00   1.0000e+00
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```

- Real roots become complex after deflation.

```
>>
>> bb = fliplr(b(2:5));
>>
>> rb = roots(bb); [rb;x]
ans =

   2.2888e+00 - 1.2568e-07i
   1.3894e+00 + 2.8019e-07i
  -3.3909e-01 - 4.4663e-01i
  -3.3909e-01 + 4.4663e-01i

>> roots(aa)
ans =

   2.2888e+00 + 0.0000e+00i
   1.3894e+00 + 0.0000e+00i
  -3.3909e-01 + 4.4663e-01i
  -3.3909e-01 - 4.4663e-01i
```

Stressed by choice and selection

Bisection? Fixed Point Iteration? Newton's Method?

Secant Method? Steffensen's Method? Muller's Method?

Choice and selection

- Bisection Method:
  - slow (linearly convergent);
  - always works for given interval $[a, b]$ with $f(a) \cdot f(b) < 0$.
- Fixed Point Iteration:
  - slow (linearly convergent);
  - need not work.
- Newton's Method:
  - fast (quadratically convergent);
  - needs derivatives; could get burnt (need not converge.)
- Secant Method:
  - between Bisection and Newton in speed;
  - need not converge.
- Steffensen's Method:
  - faster than Secant (quadratically convergent);
  - hard to stop; need not converge.
- Muller's Method:
  - handles complex roots;
  - need not converge.

Brent's Method (*a.k.a.* zeroin): Motivation

- Does not need derivatives.
- (Mostly) speed of
  $\boxed{\text{Muller's Method}}$
- (Mostly) reliability of
  $\boxed{\text{Bisection Method}}$
- Real roots only

Brent's Method (*a.k.a.* zeroin): Motivation

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Zero In

Zero In Japanese cover

Brent's method

From Wikipedia, the free encyclopedia

In numerical analysis, **Brent's method** is a root-finding algorithm combining the bisection method, the secant method and inverse quadratic interpolation. It has the reliability of bisection but it can be as quick as some of the less-reliable methods. The algorithm

Brent's method

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In numerical analysis, **Brent's method** is a root-finding algorithm combining the bisection method, the secant method and inverse quadratic interpolation. It has the reliability of bisection but it can be as quick as some of the less-reliable methods. The algorithm

- Worst case cost
  - Number of iterations $= O(n^2) (\approx 3000)$, where n is number of Bisection iterations for a given tolerance.
- Strategy
  - Performs fast iteration with INVERSE QUADRATIC INTERPOLATION or SECANT METHOD when fast convergence is possible.
  - Otherwise performs BISECTION.
- A variant of Brent's Method will be programming project.