Chapter 2 Solutions of Equations in One Variable

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- A system of nonlinear equations in multi-variables has the form

$$\begin{aligned} f_1(x_1, x_2, \cdots, x_n) &= 0 \\ f_2(x_1, x_2, \cdots, x_n) &= 0 \\ \vdots \quad & \quad \vdots \\ f_m(x_1, x_2, \cdots, x_n) &= 0 \end{aligned} \tag{1}$$

- Each function f_i can be thought of as mapping a vector $\mathbf{x} = (x_1, x_2, \cdots, x_n)^T \in \mathbb{R}^n$ into $\mathbb{R}$.

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$$\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), \cdots, f_m(\mathbf{x}))^T,$$

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- The function $\mathbf{f}$ is continuous at $\mathbf{x}_0 \in D$ provided $\lim\limits_{\mathbf{x}\to\mathbf{x}_0} \mathbf{f}(\mathbf{x})$ exists and $\lim\limits_{\mathbf{x}\to\mathbf{x}_0} \mathbf{f}(\mathbf{x}) = \mathbf{f}(\mathbf{x}_0)$.
- In addition, $\mathbf{f}$ is said to be continuous on the set D, if $\mathbf{f}$ is continuous at each $\mathbf{x}$ in D. This concept is expressed by writing

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Theorem

Let f be a function from $D \subset \mathbb{R}^n$ into $\mathbb{R}$ and $\mathbf{x}_0 \in D$. If constants $\delta > 0$ and $K > 0$ exist with

$$\left|\frac{\partial f(\mathbf{x})}{\partial x_j}\right| \leq K, \texttt{ for each } j = 1, 2, \cdots, n$$

whenever $\|\mathbf{x} - \mathbf{x}_0\| < \delta$, and $\mathbf{x} \in D$, then f is continuous at $\mathbf{x}_0$.

- **the root-finding problem:** Given a function $f(x)$ in one variable x, finding a root x of an equation of the form $f(x) = 0$.
- Solution x is called a **root of equation** $f(x) = 0$, or **zero of function** $f(x)$
- Such kind of problem is known as **root finding or zero finding problem.**

2.1 The Bisection Method for Root-finding Problem in one variable

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Interval Bisection Method

- By the Intermediate Value Theorem, if

$$f \in C[a, b], \text{ and } f(a)f(b) < 0,$$

then there exists at least a point $x^* \in (a, b)$, such that $f(x^*) = 0$.

- Bisection(折半查找) or Binary-search(二分法) method begins with an initial bracket $[a, b]$, and successively reduce its length half with opposite endpoints, until the solution has been isolated as accurately as desired..
- Although the procedure will work for the case when $f(a)$ and $f(b)$ have opposite signs and maybe there is more than one root in the interval (a, b).

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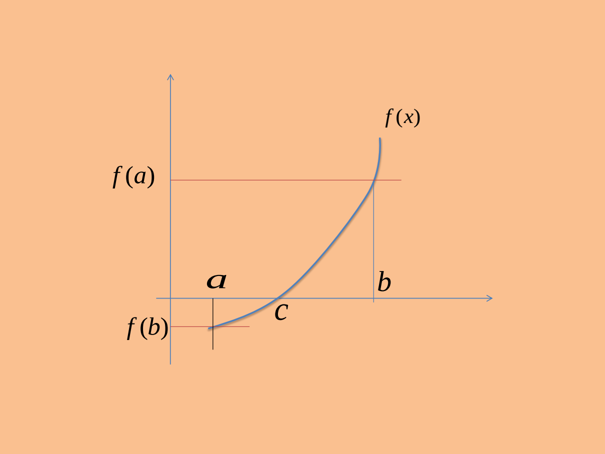
Geometric means—-Interval Bisection Method



- Let $a_1 = a, b_1 = b$ and $c_1 = (a_1 + b_1)/2$ be the midpoint of interval $[a, b]$.
- Compute $f(c_1)$, It is clear that
  - If $f(c_1) = 0$, then $c = c_1$, and c is our solution.
  - Else, if the $f(c_1)$ has the same sign as $f(a_1)$, then set $a_2 = c_1, b_2 = b_1$;
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- Continue this procedure. Suppose we have got the subinterval $[a_n, b_n]$, let $c_n = (a_n + b_n)/2 = a_n + (b_n - a_n)/2,.$
- Compute $f(c_n)$, and determine that
  - If $f(c_n) = 0$ or $|b_n - a_n| < \varepsilon$, where $\varepsilon > 0$ is small enough, then stop and output the solution as $c = c_n$.
  - Otherwise, if $f(c_n)f(a_n) < 0$, then set $a_{n+1} = a_n, b_{n+1} = c_n$, else set $a_{n+1} = c_n, b_{n+1} = b_n$
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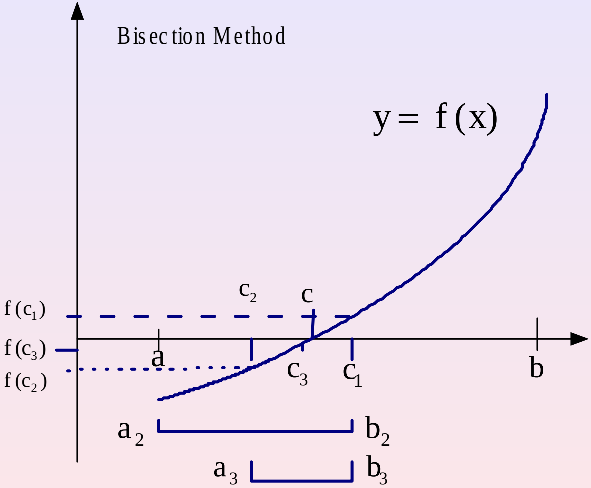
Geometric Means



Algorithm 2.1: Bisection Algorithm

INPUT endpoints a, b,; tolerance TOL; maximum number of iterations N.

OUTPUT approximate solution c or message of failure.

Step 1 Set $k = 1, FA = f(a)$;

Step 2 While $k \leq N$, do Steps 3-6

- Step 3 Set $c = a + (b - a)/2$; and compute $FC = f(c)$.
- Step 4 If $FC = 0$ or $|b - a|/2 < TOL$, then output c, (Procedure complete successfully.) Stop!
- Step 5 If $FA \cdot FC < 0$, then set $b = c$; else set $a = c$
- Step 6 Set $k = k + 1$.

Step 7 OUTPUT "Method failed after N iterations." STOP.

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Theorem

Suppose that $f \in C[a, b]$, and $f(a)f(b) < 0$. The Bisection method generates a sequence $\{p_n\}_1^\infty$ approximating a zero point p of f with

$$|p_n - p| \leq \frac{b-a}{2^n}, n \geq 1. \blacksquare$$

Proof:

- By the procedure, we know that

$$\begin{aligned} |b_1 - a_1| &= |b - a|, \\ |b_2 - a_2| &= |b_1 - a_1|/2 = |b - a|/2, \\ \cdots & \quad \cdots \\ |b_n - a_n| &= |b_{n-1} - a_{n-1}|/2 = |b - a|/2^{n-1}, \end{aligned}$$

- Since $p_n = (a_n + b_n)/2$ and $p \in (a_n, p_n]$ or $p \in [p_n, b_n)$ for all $n \geq 1$, it follows that

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Remarks on Bisection method

- Other Stopping Criteria for Iteration procedures with a given tolerance $\varepsilon > 0$:

$$
\begin{aligned}
|p_n - p_{n-1}| &< \varepsilon \\
\frac{|p_n - p_{n-1}|}{|p_n|} &< \varepsilon \\
|f(p_n)| &< \varepsilon
\end{aligned}
$$

Remarks on Bisection method

- Since

$$|p_n - p| \leq \frac{|b_n - a_n|}{2} = \frac{|b - a|}{2^n}$$

- The Sequence $\{p_n\}_{n=1}^{\infty}$ converges to p with rate of convergence $O(\frac{1}{2^n})$, that is

$$p_n = p + O(\frac{1}{2^n})$$

- Bisection is certain to converge, but does so slowly
- Given starting interval $[a, b]$, length of interval after k iterations is $(b-a)/2^k$, so achieving error tolerance of ε $(\frac{(b-a)}{2^k} < \varepsilon)$ requires $k \approx [\log_2^{\frac{b-a}{\varepsilon}}]$ iterations, regardless of function f involved.

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- **Fixed point** of given function $g : \mathbb{R} \to \mathbb{R}$ is value x^* such that $x^* = g(x^*)$
- Many iterative methods for solving nonlinear equations use fixed-point iteration scheme of form

$$x_{k+1} = g(x_k)$$

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Fixed Point Method

- This kind of method is also called **functional iteration**, since function g is applied repeatedly to initial starting value x_0
- For given equation $f(x) = 0$, there may be many equivalent fixed-point problems $x = g(x)$ with different choices for g. For example, as $g(x) = x - f(x)$ or as $g(x) = x + 3f(x)$.
- Conversely, if the function g has a fixed point at p, then the function defined by $f(x) = x - g(x)$ has a zero at p.

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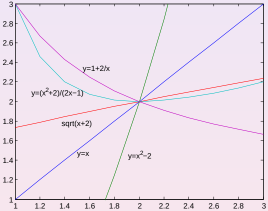
- Conversely, if the function g has a fixed point at p, then the function defined by $f(x) = x - g(x)$ has a zero at p.

If $f(x) = x^2 - x - 2$, it has two roots $x^* = 2$ and $x^* = -1$. Then fixed points of each of functions

1. $g(x) = x^2 - 2$
2. $g(x) = \sqrt{x+2}$
3. $g(x) = 1 + \frac{2}{x}$
4. $g(x) = \frac{x^2+2}{2x-1}$

are solutions to equation $f(x) = 0$.

Examples for Fixed Point Problems



- To approximate the fixed point of a function $g(x)$, we choose an initial approximation p_0, and generate the sequence $\{p_n\}_{n=0}^{\infty}$ by letting

$$\begin{cases} \texttt{Given} \quad p_0 \\ p_n = g(p_{n-1}), n = 0, 1, \cdots , \end{cases}$$

  for each $n \geq 1$.
- If the sequence $\{p_n\}_{n=0}^{\infty}$converges to p and $g(x)$ is continuous, then we have

$$p = \lim_{n\to\infty} p_n = \lim_{n\to\infty} g(p_n) = g(\lim_{n\to\infty} p_n) = g(p).$$

  and a solution to $x = g(x)$ is obtained.
- This technique is called **fixed point iteration(or functional iteration)**.

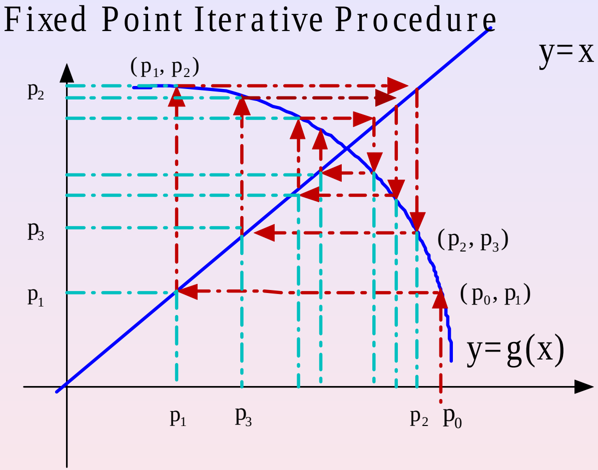


Fig.2-3. Fixed point iteration procedure.(a)

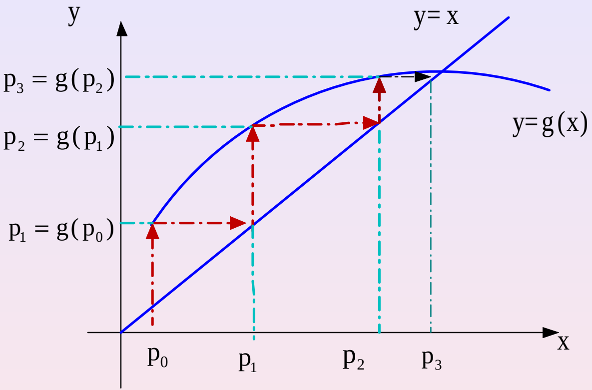


Fig.2-3. Fixed point iteration procedure.(b)

ALGORITHM 2.2 Fixed-Point Iteration Method

INPUT Initial approximation p_0, tolerance TOL,
Maximum number of iteration N.

OUTPUT approximation solution p or message of failure.

Step 1 Set $n = 1$.

Step 2 While $n \leq N$, do Step3-6.

Step 3 Set $p = g(p_0)$.

Step 4 If $|p - p_0| < TOL$ then Output p;
(Procedure completed successfully.),
STOP.

Step 5 Set $n = n + 1, p_0 = p$.

Step 6 Output 'Method failed after N iterations,
$N =$',N); (Procedure completed unsuccessfully.),
STOP.

Sufficient Conditions for the Existence and Uniqueness of a Fixed Point

THEOREM 2.2:

- a. If $g(x) \in C[a, b]$ and $g(x) \in [a, b]$ for all $x \in [a, b]$, then $g(x)$ has a fixed point in $[a, b]$.
- b. If, in addition, $g'(x)$ exists on (a, b), and a positive constant $k < 1$ exists with $|g'(x)| \leq k$, for all $x \in (a, b)$.

  Then the fixed point in $[a, b]$ is unique.■

Proof of Theorem: Existence

- If $g(a) = a$ or $g(b) = b$, then $g(x)$ has a fixed point at an endpoint.
- Suppose not, then it must be true that $g(a) > a$ and $g(b) < b$.
- Thus the function $h(x) = g(x) - x$ is continuous on $[a, b]$, and we have

$$h(a) = g(a) - a > 0, h(b) = g(b) - b < 0.$$

- The Intermediate Value Theorem implies that there exists $p \in (a, b)$ for $h(x) = g(x) - x$ which $h(p) = 0$.
- Thus $g(p) - p = 0$, and p is a fixed point of $g(x)$.

Uniqueness

- Suppose , in addition, that $|g'(x)| \leq k < 1$ and that p and q are both fixed points in $[a, b]$ with $p \neq q$.
- Then by the Mean Value Theorem, a number ξ exists between p and q, and hence in $[a, b]$, with

$$\frac{g(p) - g(q)}{p - q} = g'(\xi).$$

- Then

$$|p-q| = |g(p)-g(q)| = |g'(\xi)||p-q| \leq k|p-q| < |p-q|,$$

which is a contradiction.
- So $p = q$, and the fixed point in $[a, b]$ is unique. ■■

THEOREM 2.3 (Fixed-Point Theorem)

- Let $g \in C[a, b]$ and $g(x) \in [a, b]$ for all x in $[a, b]$.
- Suppose, in addition, that $g'(x)$ exists on (a, b) and a positive constant $k < 1$ exists with $|g'(x)| \leq k$, for all $x \in (a, b)$.
- Then for any number $p_0 \in [a, b]$, the sequence $\{p_n\}_0^\infty$ defined by

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

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

Proof of Theorem 2.3:

- Since the function $g(x)$ satisfies the all basic conditions that a unique fixed point existed, so by the theorem 2.2, we know that a unique fixed point p exists in $[a, b]$.
- Since $g(x)$ maps $[a, b]$ into itself, the sequence $\{p_n\}_0^\infty$ is defined for all $n \geq 0$, and $p_n \in [a, b]$ for all n.
- Using the fact that $|g'(x)| \leq k$ and the Mean Value Theorem, we have

$$\begin{aligned} |p_n - p| &= |g(p_{n-1}) - g(p)| = |g'(\xi)||p_{n-1} - p| \\ &\leq k|p_{n-1} - p|, \end{aligned}$$

where $\xi \in (a, b)$.

- Applying this inequality inductively gives

$$\begin{aligned} |p_n - p| &\leq k|p_{n-1} - p| \leq k^2|p_{n-2} - p| \leq \cdots \\ &\leq k^n|p_0 - p|. \end{aligned}$$

- Since $k < 1$,

$$\lim_{n\to\infty} |p_n - p| \leq \lim_{n\to\infty} k^n|p_0 - p| = 0,$$

and $\{p_n\}_0^\infty$ converges to p.$\blacksquare$.

Corollary 2.4

If $g(x)$ satisfies the hypotheses of Theorem 2.3, bounds for the error involved in using p_n to approximate p are given by

$$|p_n - p| \leq k^n \max\{p_0 - a, b - p_0\}$$

and

$$|p_n - p| \leq \frac{k^n}{1-k}|p_1 - p_0|, \text{for all} n \geq 1. \blacksquare$$

Proof:

- The first bound can be derived as follows:

$$|p_n - p| \le k^n |p_0 - p| \le k^n \max\{p_0 - a, b - p_0\},$$

- Since $p \in [a, b]$,the next inequality can be given as

$$\begin{aligned}
|p_n - p_{n-1}| &\le |g(p_{n-1}) - g(p_{n-2})| \\
&\le k|p_{n-1} - p_{n-2}| \\
&\le \cdots\cdots \\
&\le k^{n-1}|p_1 - p_0|.
\end{aligned}$$

- Let $m > n$, then we have

$$\begin{aligned} |p_m - p_n| &\leq |p_m - p_{m-1}| + |p_{m-1} - p_{m-2}| \\ &\quad + \cdots + |p_{n+1} - p_n| \\ &\leq (k^{m-1} + k^{m-2} + \cdots + k^n)|p_1 - p_0| \\ &\leq k^n(1 + k + \cdots + k^{m-n-1})|p_1 - p_0| \end{aligned}$$

- Let $m \to \infty$, and since the sequence $\{p_m\}_0^\infty$ converges to the fixed point p, we have

$$\begin{aligned} \lim_{m\to\infty} |p_m - p_n| &= |p - p_n| \\ &\leq k^n |p_1 - p_0| \sum_{i=0}^{\infty} k^i \\ &= \frac{k^n}{1-k}|p_1 - p_0|. \blacksquare \end{aligned}$$

The Newton-Raphson (or simply Newton's) method is one of the most powerful and well-known numerical methods for solving a root-finding problem

$$f(x) = 0.$$

- Suppose that $f \in C^2[a, b]$, and x^* is a solution of $f(x) = 0$.
- Let $\bar{x} \in [a, b]$ be an approximation to x^* such that $f'(\bar{x}) \neq 0$ and $|\bar{x} - x^*|$ is "small".
- Consider the first Taylor polynomial for $f(x)$ expanded about $\bar{x}$,

$$f(x) = f(\bar{x}) + (x - \bar{x})f'(\bar{x}) + \frac{(x - \bar{x})^2}{2} f''(\xi(x)).$$

where $\xi(x)$ lies between x and $\bar{x}$.

Newton's Method,Continued

- Since $f(x^*) = 0$, let $x = x^*$ in this equation, and gives

$$0 = f(x^*) = f(\bar{x}) + (x^* - \bar{x})f'(\bar{x}) + \frac{(x^* - \bar{x})^2}{2} f''(\xi(p)).$$

- Newton's method is derived by assuming that since $|x^* - \bar{x}|$ is small, thus the term involving $(x^* - \bar{x})^2$ is much smaller.
- Omit the last term, and gives

$$0 = f(x^*) \approx f(\bar{x}) + (x^* - \bar{x})f'(\bar{x}),$$

- Solving for x^* in this equation gives

$$x^* \approx \bar{x} - \frac{f(\bar{x})}{f'(\bar{x})}$$

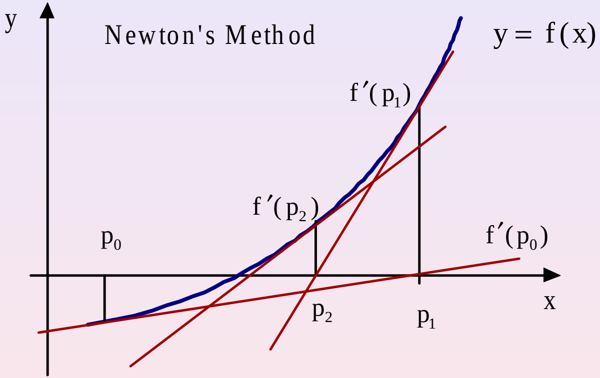
I. The Newton-Raphson Method–牛顿法或切线法

- Starts with an initial approximation x_0
- Defined iteration scheme by

$$x_n = x_{n-1} - \frac{f(x_{n-1})}{f'(x_{n-1})}, \forall n \geq 1$$

- This scheme generates the sequence $\{x_n\}_0^\infty$

Geometric Explanation for Newton's Method



ALGORITHM 2.3 Newton-Raphson Algorithm

To find a solution to $f(x) = 0$ given the differentiable function f and an initial approximation p_0:

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

OUTPUT approximate solution p or message of failure.

Step 1 Let $i = 1$.

Step 2 While $i \leq N$, do step 3-5.

Step 3 Set $p = p_0 - f(p_0)/f'(p_0)$. (Compute Pi')

Step 4 If $|p - p_0| < TOL$ then OUTPUT (p); (Procedure completed successfully.) STOP.

Step 5 Set $i = i + 1, p_0 = p$.

Step 6 OUTPUT ('Method failed after N_0 iterations, $'N =', N$); (Procedure completed unsuccessfully.) STOP.

THEOREM 2.5

- Let $f \in C^2[a, b]$.
- If $p \in [a, b]$ is such that $f(p) = 0$ and $f'(p) \neq 0$,
- then there exists a $\delta > 0$ such that Newton's method generates a sequence $\{p_n\}_1^\infty$ converging to p for any initial approximation $p_0 \in [p - \delta, p + \delta]$. ■

Proof of Theorem 2.5

- The proof is based on analyzing Newton's method as the functional iteration scheme $p_n = g(p_{n-1})$, for $n \geq 1$, with

$$g(x) = x - f(x)/f'(x).$$

- Let k be any number in $(0, 1)$.
- We first find an interval $[p-\delta, p+\delta]$ that g maps into itself, and $|g'(x)| \leq k$ for all $x \in (p-\delta, p+\delta)$
- Since $f'(p) \neq 0$ and f' is continuous, there exists $\delta_1 > 0$ such that $f'(x) \neq 0$ for $x \in [p-\delta_1, p+\delta_1] \subset C[a.b]$.
- Thus, g is defined and continuous on $[p-\delta_1, p+\delta_1]$.

Proof: Continued

- Also,

$$g'(x) = 1 - \frac{(f'(x)f'(x) - f(x)f''(x))}{[f'(x)]^2} = \frac{f(x)f''(x)}{[f'(x)]^2}$$

for $x \in [p - \delta_1, p + \delta_1]$, and since $f \in C^2[a, b]$, we have $g \in C^1[p - \delta_1, p + \delta_1]$.

- By assumption, $f(p) = 0$, so

$$g'(p) = f(p)f''(p)/[f'(p)]^2 = 0.$$

- Since g' is continuous and $0 < k < 1$, there exists a δ, with $0 < \delta < \delta_1$ and

$$|g'(x) \leq k, \quad \forall x \in [p - \delta, p + \delta].$$

- It remains to show that

$$g \in [p - \delta, p + \delta] \mapsto [p - \delta, p + \delta].$$

- If $x \in [p-\delta, p+\delta]$, the Mean Value Theorem implies that, for some number ξ between x and p, $|g(x) - g(p)| = |g'(\xi)|x - p|$.
- So

$$\begin{aligned} |g(x) - p| &= |g(x) - g(p)| = |g'(\xi)||x - p| \\ &\leq k|x - p| < |x - p|. \end{aligned}$$

- Since $x \in [p-\delta, p+\delta]$, it follows that $|x - p| < \delta$ and that $|g(x) - p| < \delta$.
- This result implies that $g \in [p-\delta, p+\delta] \mapsto [p-\delta, p+\delta]$.
- All the hypotheses of the Fixed-Point Theorem are now satisfied for $g(x) = x - f(x)/f'(x)$, so the sequence $\{p_n\}_{n=1}^{\infty}$ defined by

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

converges to p for any $p_0 \in [p-\delta, p+\delta]$. ■

- Use Newton's method to find root of equation

$$f(x) = x^2 - 4\sin(x) = 0$$

- Derivative is

$$f'(x) = 2x - 4\cos(x).$$

- So iteration scheme is

$$x_{k+1} = x_k - \frac{x_k^2 - 4\sin(x_k)}{2x_k - 4\cos(x_k)}$$

Taking $x_0 = 3$ as starting value, we obtain

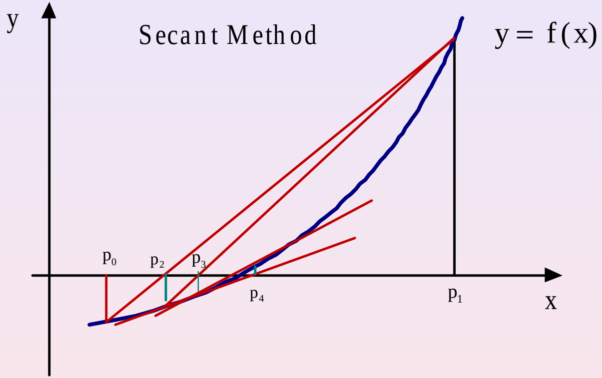
k	x	$f(x)$	$f'(x)$
0	3.000000	8.435520	9.959970
1	2.153058	1.294772	6.505771
2	1.954039	0.108438	5.403795
3	1.933972	0.001152	5.288919
4	1.933754	0.000000	5.287670

- **Remark:** For Newton's method, each iteration requires evaluation of both **function** $(f(x_k))$ and its **derivative**$(f'(x_k))$, which may be inconvenient or expensive.
- **Improvement:** Derivative is approximated by finite difference using two successive iterates, so iteration becomes

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

- This method is known as **secant method**.

Secant Method, continued



Example: Secant Method

Using Secant's method to find a root of equation

$$f(x) = x^2 - 4\sin(x) = 0$$

Taking $x = 1, 3$ as starting values, we obtain

k	x_k	$f(x_k)$
0	1.0000	−2.3659
1	3.0000	8.4355
2	1.4381	−1.8968
3	1.7248	−0.9777
4	2.0298	0.5343
5	1.9220	−0.0615
6	1.9332	−0.0031
7	1.9338	0.0000

Secant Algorithm 2.4

INPUT: initial approximations p_0, p_1; tolerance TOL; maximum number of iterations N_0.

OUTPUT: approximate solution p or message of failure.

Step 1 Set $i = 1$; $q_0 = f(p_0)$; $q_1 = f(p_1)$.

Step 2 While $i \leq N_0$, do step 3-6.

  Step 3 Set $p = p_1 - q_1(p_1 - p_0)/(q_1 - q_0)$. (Compute p_i),

  Step 4 If $|p - p_1| < TOL$ then OUTPUT (p); (Procedure completed successfully.) STOP.

  Step 5 Set $i = i + 1$.

  Step 6 Set

  $$p_0 = p_1, p_1 = p; q_0 = q_1, q_1 = f(p);$$

  (Update p_0, q_0, p_1, q_1.)

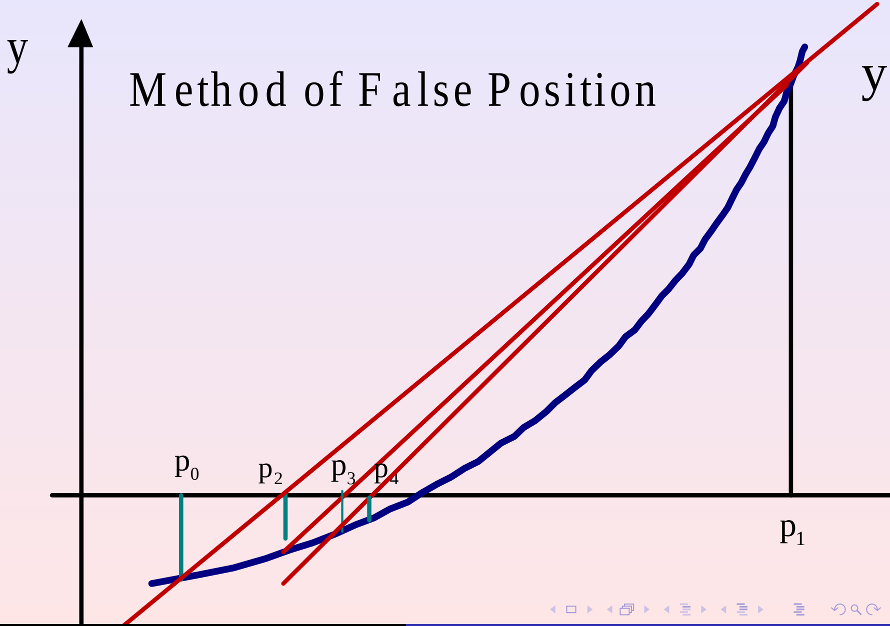
Step 7 OUTPUT ('Method failed after N_0 iterations, $N_0 =$', N_0); (Procedure completed unsuccessfully.) STOP.

III. Method of False Position–错位法

- To find a solution to $f(x) = 0$ for a given the continuous function f on the interval $[p_0, p_1]$, where $f(p_0)$ and $f(p_1)$ have opposite signs

$$f(p_0)f(p_1) < 0.$$

- The approximation p_2 is chosen in same manner as in Secant Method, as the x-intercept of the line joining $(p_0, f(p_0))$ and $(p_1, f(p_1))$.
- To decide which Secant Line to use to computer p_3, we need to check $f(p_2) \cdot f(p_1)$ or $f(p_2) \cdot f(p_0)$.
- If this value is negative, then p_1, p_2 bracket a root, and we choose p_3 as the x-intercept of the line joining $(p_1, f(p_1))$ and $(p_2, f(p_2))$.
- In a similar manner, we can get a sequence $\{p_n\}_2^\infty$ which approximates to the root.


Method of False Position
y
y
p0
p2
p3
p4
p1

False Position Algorithm 2.5

INPUT initial approximations p_0, p_1; tolerance TOL; maximum number of iterations N_0.
OUTPUT] approximate solution p or message of failure.

Step 1 Set $i = 2$; $q_0 = f(p_0)$; $q_1 = f(p_1)$.

Step 2 While $i \leq N_0$, do Step 3-6.

- Step 3 Set $p = p_1 - q_1(p_1 - p_0)/(q_1 - q_0)$. (Compute p_i),
- Step 4 If $|p - p_1| < TOL$ then OUTPUT (p); (Procedure completed successfully.) STOP.
- Step 5 Set $i = i + 1, q = f(p)$.
- Step 6 If $q.q_1 < 0$ then set $p_0 = p, q_0 = q$; else $p_1 = p, q_1 = q$.

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

In this section , we will investigate

- **The rate of convergence** of a sequence;
- **The order of convergence** of functional iteration schemes;
- **Ways of accelerating the convergence of Newton's method.**

Definition for measuring the rate of a sequence convergence.

Definition 2.6

- Suppose $\{p_n\}_{n=0}^{\infty}$ 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 $\{p_n\}_{n=0}^{\infty}$ **converges to** p **of order** α**, with asymptotic error constant** λ.$\blacksquare$

- An iterative technique of the form

$$p_n = g(p_{n-1})$$

is said to be **of order** α if the sequence $\{p_n\}_{n=0}^{\infty}$ (generated by $p_n = g(p_{n-1}), n = 1, 2, \cdots$) converges to the solution $p = g(p)$ of order α.

- In general, a sequence with a high order of convergence converges more rapidly than a sequence with a lower order.
- The asymptotic constant affects the speed of convergence but is not as important as the order.

Two cases of order are given special attention.

(I) If $\alpha = 1$, the sequence is **linearly convergent**.

(II) If $\alpha = 2$, the sequence is **quadratically convergent**.

Example 3

- Suppose two sequences $\{p_n\} \mapsto 0$ and $\{q_n\} \mapsto 0$
- Further, we also suppose that

$$\lim_{n\to\infty} \frac{|p_{n+1}|}{|p_n|} = 0.5, \quad \lim_{n\to\infty} \frac{|q_{n+1}|}{|q_n|^2} = 0.5.$$

- Suppose also, for simplicity, that

$$\frac{|p_{n+1}|}{|p_n|} \approx 0.5, \text{and} \frac{|q_{n+1}|}{|q_n|^2} \approx 0.5.$$

- These mean that

$$\begin{aligned} |p_n - 0| &= |p_n| \approx 0.5|p_{n-1}| \approx 0.5^2|p_{n-2}| \\ &\approx \cdots \approx 0.5^n|p_0|; \\ |q_n - 0| &= |q_n| \approx 0.5|p_{n-1}|^2 \approx 0.5 \times (0.5|q_{n-2}|^2)^2 \\ &= 0.5^3|q_{n-2}|^4 \approx \cdots \approx 0.5^{2^n-1}|p_0|^{2^n}. \end{aligned}$$

- Quadratical convergent sequence generally converges more rapidly than those that converge only linearly.

Example 3

- Suppose two sequences $\{p_n\} \mapsto 0$ and $\{q_n\} \mapsto 0$
- Further, we also suppose that

$$\lim_{n\to\infty} \frac{|p_{n+1}|}{|p_n|} = 0.5, \quad \lim_{n\to\infty} \frac{|q_{n+1}|}{|q_n|^2} = 0.5.$$

- Suppose also, for simplicity, that

$$\frac{|p_{n+1}|}{|p_n|} \approx 0.5, \text{and} \frac{|q_{n+1}|}{|q_n|^2} \approx 0.5.$$

- These mean that

$$\begin{aligned} |p_n - 0| &= |p_n| \approx 0.5|p_{n-1}| \approx 0.5^2|p_{n-2}| \\ &\approx \cdots \approx 0.5^n|p_0|; \\ |q_n - 0| &= |q_n| \approx 0.5|p_{n-1}|^2 \approx 0.5 \times (0.5|q_{n-2}|^2)^2 \\ &= 0.5^3|q_{n-2}|^4 \approx \cdots \approx 0.5^{2^n-1}|p_0|^{2^n}. \end{aligned}$$

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- Suppose two sequences $\{p_n\} \mapsto 0$ and $\{q_n\} \mapsto 0$
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- Suppose also, for simplicity, that

$$\frac{|p_{n+1}|}{|p_n|} \approx 0.5, \text{ and } \frac{|q_{n+1}|}{|q_n|^2} \approx 0.5.$$

- These mean that

$$\begin{aligned} |p_n - 0| &= |p_n| \approx 0.5|p_{n-1}| \approx 0.5^2|p_{n-2}| \\ &\approx \cdots \approx 0.5^n|p_0|; \\ |q_n - 0| &= |q_n| \approx 0.5|p_{n-1}|^2 \approx 0.5 \times (0.5|q_{n-2}|^2)^2 \\ &= 0.5^3|q_{n-2}|^4 \approx \cdots \approx 0.5^{2^n-1}|p_0|^{2^n}. \end{aligned}$$

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Example 3

- Suppose two sequences $\{p_n\} \mapsto 0$ and $\{q_n\} \mapsto 0$
- Further, we also suppose that

$$\lim_{n\to\infty} \frac{|p_{n+1}|}{|p_n|} = 0.5, \quad \lim_{n\to\infty} \frac{|q_{n+1}|}{|q_n|^2} = 0.5.$$

- Suppose also, for simplicity, that

$$\frac{|p_{n+1}|}{|p_n|} \approx 0.5, \text{and} \frac{|q_{n+1}|}{|q_n|^2} \approx 0.5.$$

- These mean that

$$\begin{aligned} |p_n - 0| &= |p_n| \approx 0.5|p_{n-1}| \approx 0.5^2|p_{n-2}| \\ &\approx \cdots \approx 0.5^n|p_0|; \\ |q_n - 0| &= |q_n| \approx 0.5|p_{n-1}|^2 \approx 0.5 \times (0.5|q_{n-2}|^2)^2 \\ &= 0.5^3|q_{n-2}|^4 \approx \cdots \approx 0.5^{2^n-1}|p_0|^{2^n}. \end{aligned}$$

- Quadratical convergent sequence generally converges more rapidly than those that converge only linearly.

THEOREM 2.7

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

$$|g'(x)| \leq k,$$

for all $x \in (a,b)$.
- If $g'(p) \neq 0$, then for any number p_0 in $[a,b]$ the sequence $p_n = g(p_{n-1})$, for $n \geq 1$, converges **only linearly to the unique fixed point** p in $[a,b]$. ■

Proof of Theorem 2.7:

- We know from the Fixed-Point Theorem 2.3 in Section 2.2 that the sequence converges to p.
- Since g' exists on $[a, b]$, we can apply the Mean Value Theorem to g to show that for any n,

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

  where ξ_n is between p_n and p.
- Since $\{p_n\}_{n=0}^{\infty}$ converges to p, and ξ_n is between p_n and p, thus $\{\xi_n\}_{n=0}^{\infty}$ also converges to p.
- By the known condition, g' is continuous on [a, b], so we have

$$\lim_{n\to\infty} g'(\xi_n) = g'(p).$$

Continued

- Thus,

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

  and

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

- Hence, fixed-point iteration exhibits linear convergence with asymptotic error constant $|g'(p)|$ whenever $g'(p) \neq 0$.■

- Theorem 2.7 implies that higher-order convergence for fixed-point methods can occur only when $g'(p) = 0$.
- The next result describes additional conditions that ensure the quadratic convergence we seek.

THEOREM 2.8

- Let p be a solution of the equation $x = g(x)$.
- Suppose that $g'(p) = 0$ and g'' is continuous and strictly bounded by M on an open interval I containing p.
- Then there exists a $\delta > 0$ such that, for $p_0 \in [p - \delta, p + \delta]$, the sequence defined by $p_n = g(p_{n-1})$, when $n \geq 1$, **converges at least quadratically to** p.
- Moreover, for sufficiently large values of n,

$$|p_{n+1} - p| < \frac{M}{2}|p_n - p|^2. \blacksquare$$

Proof of Theorem 2.8:

- Since $g'(p) = 0$ and $g''(x)$ is continuous on the open interval I, so we can choose a positive k $(0 < k < 1)$ and $\delta > 0$ such that on the interval $[p-\delta, p+\delta]$, contained in I, we have $|g'(x)| \leq k$ and g'' continuous.
- Since $|g'(x)| \leq k < 1$, the argument used in the proof of Theorem 2.5 in Section 2.3 shows that the terms of the sequence $\{p_n\}_{n=0}^{\infty}$ are contained in $[p-\delta, p+\delta]$.
- Expanding $g(x)$ in a linear Taylor polynomial for $x \in [p-\delta, p+\delta]$ gives

$$g(x) = g(p) + g'(p)(x-p) + \frac{g''(\xi)}{2}(x-p)^2,$$

where ξ lies between x and p.
- The hypotheses $g(p) = p$ and $g'(p) = 0$ imply that

$$g(x) = p + \frac{g''(\xi)}{2}(x-p)^2$$

- In particular, when $x = p_n$,

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

with ξ_n between p_n and p.

- Thus

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

- Since $|g'(x)| \leq k < 1$ on $[p-\delta, p+\delta]$ and g maps $[p-\delta, p+\delta]$ into itself, it follows from the Fixed-Point Theorem that $\{p_n\}_{n=0}^{\infty}$ converges to p.
- But ξ_n is between p and p_n for each n, so $\{\xi_n\}_{n=0}^{\infty}$ also converges to p, and, since g'' is continuous,

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

- This result implies that the sequence $\{p_n\}_{n=0}^{\infty}$ is quadratically convergent if $g''(p) \neq 0$ and of higher-order convergence if $g''(p) = 0$. Since g'' is strictly bounded by M on the interval $[p-\delta, p+\delta]$, this also implies that for sufficiently large values of n,

$$|p_{n+1} - p| < \frac{M}{2}|p_n - p|^2. \blacksquare$$

Problem? How to construct a fixed point problem $x = g(x)$ to be quadratically convergent associated with a root finding problem $f(x) = 0$?

- Let $g(x)$ be in the form

$$g(x) = x - \phi(x)f(x),$$

- For the iteration procedure derived from $g(x)$ to be quadratically convergent, we need to have $g'(p) = 0$.
- Since

$$g'(x) = 1 - \phi'(x)f(x) - \phi(x)f'(x).$$

  Let $x = p$, we have $g'(p) = 1 - \phi(p)f'(p)$, and $g'(p) = 0$ if only if $\phi(p) = 1/f'(p)$.
- A reasonable approach is to let $\phi(x) = 1/f'(x)$, which is the **Newton's method**.

Definition 2.9

A solution p of $f(x) = 0$ is a **zero of multiplicity** m of $f(x)$ if for $x \neq p$, we can write

$$f(x) = (x - p)^m q(x),$$

where

$$\lim_{x \to p} q(x) \neq 0. \blacksquare$$

THEOREM 2.10

$f \in C^1[a, b]$ has a **simple zero** at p in (a, b) if and only if $f(p) = 0$, but $f'(p) \neq 0$. $\blacksquare$

Proof of Theorem 2.10

- If f has a simple zero at p, then

$$f(p) = 0$$

and

$$f(x) = (x - p)q(x),$$

where

$$\lim_{x \to p} q(x) \neq 0.$$

- Since $f \in C^1[a, b]$,

$$\begin{aligned} f'(p) &= \lim_{x \to p} f'(x) = \lim_{x \to p} [q(x) + (x - p)q'(x)] \\ &= \lim_{x \to p} q(x) \neq 0. \end{aligned}$$

- Conversely, if $f(p) = 0$, but $f'(p) \neq 0$, expand f in a zeroth Taylor polynomial about p.
- Then

$$f(x) = f(p) + f'(\xi(x))(x-p) = f'(\xi(x))(x-p),$$

where $\xi(x)$ is between x and p.
- Since $f \in C^1[a, b]$,

$$\lim_{x \to p} f'(\xi(x)) = f'(\lim_{x \to p} \xi(x)) = f'(p) \neq 0.$$

- Letting $q = f' \circ \xi$ gives $f(x) = (x-p)q(x)$, where $\lim_{x \to p} q(x) \neq 0$.
- Thus f has a simple zero at p. □□□

THEOREM 2.11

The function $f \in C^m[a,b]$ has a zero of multiplicity m at p if and only if

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

but

$$f^{(m)}(p) \neq 0. \blacksquare$$

Method to handle multiple root finding problems:

Define a function μ by

$$\mu(x) = f(x)/f'(x).$$

If p is a zero of multiplicity m and

$$f(x) = (x-p)^m q(x),$$

then

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

also has a zero at p.

- However, since $q(p) \neq 0$,

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

so p is a zero of multiplicity 1 of $\mu(x)$.

- Newton's method can be applied to the function μ to give

$$\begin{aligned} g(x) &= x - \frac{\mu(x)}{\mu'(x)} \\ &= x - \frac{f(x)/f'(x)}{[f'(x)^2 - f(x)f''(x)]/f'(x)^2}, \end{aligned}$$

or

$$g(x) = x - \frac{f(x)f'(x)}{[f'(x)]^2 - f(x)f''(x)}.$$

1. Newton's method transforms nonlinear equation $f(x) = 0$ into fixed-point problem $x = g(x)$, where $g(x) = x - f(x)/f'(x)$ and hence
$$g'(x) = f(x)f''(x)/(f'(x))^2$$
2. If p is simple root (
$$\texttt{i.e.,} f(p) = 0 \text{ and } f'(p) \neq 0,$$
then $g'(p) = 0$, thus Convergence rate of **Newton's method** for simple root is therefore **quadratic** $(r = 2)$
3. But iterations must **start close enough to root** to converge.

Multiple Root Problem with Newton's Method

- Suppose equation $f(x)$ has m multiplicity at p, then we can rewrite it as $f(x) = (x-p)^m q(x)$.
- Thus by Newton's method, we have

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

- So

$$g(p) = p$$

and

$$g'(p) = 1 - \frac{q(p)}{mq(p)} = 1 - \frac{1}{m} \neq 0.$$

- **Conclusion:**
  - For a simple root, the Newton's method has quadratic convergence rate;
  - For multiple root,the Newton's method is only linear convergent.

- To avoid multiple root, we define a new function μ by
$$\mu(x) = f(x)/f'(x).$$
- If p is a zero of multiplicity m and $f(x)$ then we can rewrite it as
$$\begin{aligned}\mu(x) &= \frac{(x-p)^m q(x)}{m(x-p)^{m-1}q(x) + (x-p)^m q'(x)} \\ &= (x-p)\frac{q(x)}{mq(p) + (x-p)q'(x)},\end{aligned}$$
also has a zero at p.

- However, since $q(p) \neq 0$,

$$\mu'(p) = \frac{q(p)}{mq(p) + (p-p)q'(p)} = \frac{1}{m} \neq 0,$$

so p is a zero of multiplicity 1 of $\mu(x)$.

- Newton's method can be applied to the function μ to give

$$g(x) = x - \frac{\mu(x)}{\mu'(x)} = x - \frac{f(x)/f'(x)}{[f'(x)^2 - f(x)f''(x)]/f'(x)^2},$$

or

$$g(x) = x - \frac{f(x)f'(x)}{f'(x)^2 - f(x)f''(x)}.$$

- Thus the convergence rate is also quadratic.

Convergence Rate OF Fixed Point

- Let p be a fixed point, p_{k+1} be the approximate solution at the kth iteration, generated by

$$p_{k+1} = g(p_k),$$

then the error can be described as

$$e_{k+1} = p_{k+1} - p = g(p_k) - g(p).$$

- Suppose $g(x) \in C^1[a, b]$, then by the Mean Value Theorem, there is a point θ_k between p_k and p, such that

$$\begin{aligned} e_{k+1} &= p_{k+1} - p = g(p_k) - g(p) \\ &= g'(\theta_k)(p_k - p) \\ &= g'(\theta_k) e_k \end{aligned}$$

- Since $|g'(p)| < 1$, and the starting iteration close enough to p, we can assure that there exist a constant C, such that

$$|g'(\theta_k)| < C < 1, k = 0, 1, \cdots$$

- Thus we have

$$|e_{k+1}| \leq C|e_k| \leq C^2|e_{k-1}| \leq \cdots \leq C^{k+1}|e_0|.$$

- But $C < 1$ implies that $C^k \to 0$, so $e_k \to 0, k \to \infty$, and the sequence converges to the solution p.

- And we also can see that

$$\lim_{k\to\infty}\frac{|e_{k+1}|}{|e_k|}=\lim_{k\to\infty}g'(\theta_k)=g'(p)$$

So the asymptotic convergence rate is linear.

- Further if $g'(p)=0$, then by the Taylor's theorem

$$e_{k+1}=p_{k+1}-p=g(p_k)-g(p)=g''(\xi_k)(p_k-p)^2/2$$

for some ξ_k between p_k and p.

- Thus

$$\lim_{k\to\infty}\frac{|e_{k+1}|}{|e_k|^2}=\lim_{k\to\infty}\frac{|g''(\xi_k)|}{2}$$

and hence the convergence rate is **at least quadratic.**

Remarks on Convergence of Fixed-Point Iteration

1. **Local Convergent:** If $p = g(p)$ and $|g'(p)| < 1$, then there is an interval containing p such that iteration $p_{k+1} = g(p_k)$ converges to p if started with a point within that interval.
2. If $|g'(p)| > 1$, then iterative scheme **diverges** with any starting point other than p.
3. **Convergence rate** of fixed-point iteration is usually **linear**, with constant $C = |g'(p)|$
4. But if $g'(p) = 0$, then convergence rate is **at least quadratic**.

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1. **Convergence rate** of secant method is normally **superlinear,** with $r \approx 1.618$, which is lower than Newton's method.
2. Secant method need to evaluate two previous functions per iteration, there is no requirement to evaluate the derivative.
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- In this section, we consider a technique call Aitken's Δ^2 method that can be used to **accelerate the convergence of a sequence** that is linearly convergent, regardless of its origin or application.
- Suppose $\{p_n\}_{n=0}^{\infty}$ is a **linearly convergent sequence** with limit p.
- That means

$$\lim_{n\to\infty} \frac{p_{n+1}-p}{p_n-p} = \lambda, (\lambda \neq 0).$$

So when n is sufficiently large,

$$p_n - p, p_{n+1} - p, p_{n+2} - p$$

agree with the same sign as λ, and

$$\frac{p_{n+1} - p}{p_n - p} \approx \frac{p_{n+2} - p}{p_{n+1} - p}.$$

Then

$$(p_{n+1} - p)^2 \approx (p_{n+2} - p)(p_n - p),$$

so

$$\begin{aligned} & p_{n+1}^2 - 2p_{n+1}p + p^2 \\ \approx\ & p_{n+2}p_n - (p_n + p_{n+2})p + p^2 \end{aligned}$$

and

$$(p_n - 2p_{n+1} + p_{n+2})p \approx p_{n+2}p_n - p_{n+1}^2$$

Solving for p gives

$$\begin{aligned} p &\approx \frac{p_n p_{n+2} - p_{n+1}^2}{p_{n+2} - 2p_{n+1} + p_n} \\ &= \frac{p_n^2 + p_n p_{n+2} - 2p_n p_{n+1} - p_n^2 + 2p_n p_{n+1} - p_{n+1}^2}{p_{n+2} - 2p_{n+1} + p_n} \\ &= p_n - \frac{(p_{n+1} - p_n)^2}{p_{n+2} - 2p_{n+1} + p_n} \end{aligned}$$

Aitken's Δ^2 method

- Aitken's Δ^2 method is to define a new sequence $\{\hat{p}\}_{n=0}^{\infty}$:

$$\hat{p}_n = p_n - \frac{(p_{n+1} - p_n)^2}{p_{n+2} - 2p_{n+1} + p_n}$$

- We can prove that the new sequence can converge to p more rapidly than does the originally sequence $\{p_n\}_{n=0}^{\infty}$.

Definition 2.12

Given the sequence $\{p_n\}_{n=0}^{\infty}$, **the forward difference** Δp_n is defined by

$$\Delta p_n = p_{n+1} - p_n, \text{ for } \ n \geq 0.$$

Higher powers $\Delta^k p_n$ are defined recursively by

$$\Delta^k p_n = \Delta(\Delta^{k-1} p_n), \text{ for } \ k \geq 2 \blacksquare$$

- This implies that

$$
\begin{aligned}
\Delta^2 p_n &= \Delta(\Delta p_n) = \Delta(p_{n+1} - p_n) \\
&= \Delta p_{n+1} - \Delta p_n = p_{n+2} - 2p_{n+1} + p_n
\end{aligned}
$$

- By this definition, we rewrite the formula

$$\hat{p}_n = p_n - \frac{(p_{n+1} - p_n)^2}{p_{n+2} - 2p_{n+1} + p_n}$$

as more simple form

$$\hat{p}_n = p_n - \frac{(\Delta p_n)^2}{\Delta^2 p_n}$$

THEOREM 2.13

Suppose that $\{p_n\}_{n=0}^{\infty}$ is a sequence that converges linearly to limit p, and for all sufficiently large values of n, we have

$$(p_n - p)(p_{n+1} - p) > 0.$$

then the sequence $\{\hat{p}_n\}_{n=0}^{\infty}$ converges to p faster than $\{p_n\}_{n=0}^{\infty}$ in the sense that

$$\lim_{n\to\infty} \frac{\hat{p}_n - p}{p_n - p} = 0. \blacksquare$$

The proof of this theorem take as homework.

Special Case: for the sequence generated by fixed point iteration $P_{n+1} = g(P_n)$

For a fixed point iteration, the procedure of convergence accelerating can be shown as follows:

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

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

$$p_0^{(2)} = p_0^{(1)} - \frac{(\Delta p_0^{(1)})^2}{\Delta^2 p_0^{(1)}}, p_1^{(2)} = g(p_0^{(2)}), p_2^{(2)} = g(p_1^{(2)})$$

$$\cdots, \cdots, \cdots;$$

$$p_0^{(n)} = p_0^{(n-1)} - \frac{(\Delta p_0^{(n-1)})^2}{\Delta^2 p_0^{(n-1)}}, p_1^{(n)} = g(p_0^{(n)}), p_2^{(n)} = g(p_1^{(n)})$$

This procedure belongs to **Steffensen**.

Steffensen's Method:

- For a fixed iteration problem $p = g(p)$, given initial approximation p_0,.
- Let $p_0, p_1 = g(p_0), p_2 = g(p_1)$, and then

$$\hat{p}_0 = p_0 - (p_1 - p_0)^2/(p_2 - 2p_1 + p_0).$$

- Assume that $\hat{p}_0$ is a better approximation than p_2, and applies fixed point iteration to $\hat{p}_0$ instead of p_2, that is to let
- $p_0 = \hat{p}_0, p_1 = g(p_0), p_2 = g(p_1)$,
- $\hat{p}_0 = p_0 - (p_1 - p_0)^2/(p_2 - 2p_1 + p_0)$.
- ....

Steffensen Algorithm

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.

OUTPUT approximate solution p, or message of failure.

Step 1 Set i=1.

Step 2 While $i \leq N_0$, do Step 3-6.

- Step 3 Set $p_1 = g(p_0), p_2 = g(p_1), p = p_0 - (p_1 - p_0)^2/(p_2 - 2p_1 + p_0)$.
- Step 4 If $|p - p_0| < TOL$, THEN output p, STOP.
- Step 5 Set $i = i + 1$.
- Step 6 Set $p_0 = p$.

Step 7 OUTPUT (Method failed after N_0 iterations, "$N_0 =$", N_0), STOP.

Theorem 2.14

- Suppose that $x = g(x)$ has the solution p with $g'(p) \neq 1$.
- If there exists a $\delta > 0$ such that

$$g \in C^3[p-\delta, p+\delta],$$

- then Steffensen's method gives quadratic convergence for any $p_0 \in [p-\delta, p+\delta]$. $\blacksquare$

- In this section, we will discuss the root finding methods for a polynomial of order n.
- **Definition 2.14**: A Polynomial of Degree n has the form:

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

where $a_i, i = n, n-1, \cdots, 1, 0$ are coefficients of $P(x)$, and $a_n \neq 0$. ■

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THEOREM 2.15 (Fundamental Theorem of Algebra:)

If $P(x)$ is a polynomial of degree $n (n \geq 1)$, then $P(x)$ has at least one root (possibly complex) .

Corollary 2.16

If $P(x)$ is a polynomial of degree $n \geq 1$, then there exist **unique constants** $x_1, x_2, \cdots, x_k$ (possibly complex), and **positive integer** $m_1, m_2, \cdots, m_k$, such that $\sum_{i=1}^{n} m_i = n$, and

$$P(x) = a_n (x - x_1)^{m_1} (x - x_2)^{m_2} \cdots (x - x_k)^{m_k}. \blacksquare$$

Corollary 2.17

Let $P(x)$ and $Q(x)$ are polynomials of degree at most n, if $x_1, x_2, \cdots, x_k$ with $k > n$ are distinct numbers with $P(x_i) = Q(x_i), i = 1, 2, \cdots, k$, then $P(x) = Q(x)$ for all values of x.■

Proof: Since $P(x)$ and $Q(x)$ are polynomials of degree at most n. Let

$$P(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

and

$$Q(x) = b_0 + b_1 x + b_2 x^2 + \cdots + b_n x^n$$

are different polynomials of degree at most n.

- Let

$$\begin{aligned} R(x) &= P(x) - Q(x) \\ &= (a_0 - b_0) + (a_1 - b_1)x + (a_2 - b_2)x^2 \\ &\quad + \cdots + (a_n - b_n)x^n, \end{aligned}$$

then $R(x)$ is also a polynomial of degree at most n.

- As known condition, there exists $k > n$ distinct points or numbers $x_1, x_2, \cdots, x_k$, such that $R(x_i) = P(x_i) - Q(x_i) = 0$.
- This implies $R(x) \equiv 0$ for all values of x, or $P(x) = Q(x)$. ■

- To find the **roots for a polynomial** $P(x) = 0$ using the methods such as Newton's method in previous sections, we need to evaluate $P(x)$ and $P'(x)$ at specified points.
- Since both $P(x)$ and $P'(x)$ are polynomials, computational efficiency is required for evaluation of these functions.
- Horner gave a more efficient method to do this.

Example: How to find a value at a given point x_0 of $P(x_0) =?$

THEOREM 2.18

- Let

$$P(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0.$$

- If $b_n = a_n$ and

$$b_k = a_k + b_{k+1} x_0, k = n-1, n-2, \cdots, 1, 0,$$

then $b_0 = p(x_0)$.

- Moreover, if

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

then

$$P(x) = (x - x_0) Q(x) + b_0. \blacksquare$$

Proof of Theorem 2.18

- By the Definition of $Q(x)$, we have

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

- By the hypothesis,

$$
\begin{aligned}
b_n &= a_n, \\
b_{n-1} - b_n x_0 &= a_{n-1}, \\
&\cdots, \\
b_1 - b_2 x_0 &= a_1, \\
b_0 - b_1 x_0 &= a_0,
\end{aligned}
$$

- so

$$(x - x_0)Q(x) + b_0 = P(x).$$

and $P(x_0) = b_0, \blacksquare\blacksquare\blacksquare$

- Using Horner's Method to evaluate the value $P(x_0)$ of a polynomial

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

at a specified point x_0.

- This equals to find b_0.
- **Horner's Method**:

	a_n	a_{n-1}	a_{n-2}	$\cdots$	a_1	a_0
		$+$	$+$	$\cdots$	$+$	$+$
x_0		$b_n x_0$	$b_{n-1}x_0$	$\cdots$	$b_2 x_0$	$b_1 x_0$
$=$	$b_n = a_n$	b_{n-1}	b_{n-2}	$\cdots$	b_1	b_0

♦ Computing the derivative $P'(x_0)$ of $P(x)$

- Since $P(x) = (x - x_0)Q(x) + b_0$, thus differentiating with respect to x, gives

$$P'(x) = Q(x) + (x - x_0)Q'(x), \Rightarrow P'(x_0) = Q(x_0).$$

- Due to $Q(x)$ is also a polynomial of degree at most $n-1$, so Horner's Method can be used to get $Q(x_0)$, which equals to $P'(x_0)$.
- By Horner's method, since

$$Q(x) = b_n x^{n-1} + b_{n-1}x^{n-2} + \cdots + b_2 x + b_1.$$

Let $Q(x) = (x - x_0)R(x) + c_1$, where

$$R(x) = c_n x^{n-2} + c_{n-1}x^{n-3} + \cdots + c_3 x + c_2.$$

- Thus

$$
\begin{aligned}
Q(x) &= (x - x_0)R(x) + c_1 \\
&= (x - x_0)(c_n x^{n-2} + c_{n-1}x^{n-3} + \cdots \\
&\quad + c_3 x + c_2) + c_1 \\
&= c_n x^{n-1} + (c_{n-1} - c_n x_0)x^{n-2} \\
&\quad + (c_{n-2} - c_{n-1}x_0)x^{n-3} \\
&\quad + \cdots + (c_2 - c_3 x_0)x + (c_1 - c_2 x_0) \\
&= b_n x^{n-1} + b_{n-1}x^{n-2} + \cdots + b_2 x + b_1.
\end{aligned}
$$

- $\Rightarrow$

$$
\begin{aligned}
c_n &= b_n, \\
c_k &= b_k + c_{k+1}x_0, \; k = n-1, n-2, \cdots, 2, 1
\end{aligned}
$$

- And $Q(x_0) = c_1 = P'(x_0)$

To compute the value $P(x_0)$ of a polynomial

$$P(x) = a_n x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0.$$

and its derivative $P'(x_0)$.

INPUT degree n; Coefficients $a_0, a_1, a_2, \cdots, a_n$ of polynomial $P(x)$; Point x_0.

OUTPUT values of $P(x_0)$ and $P'(x_0)$.

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

Step 2 For $j = n-1, n-2, \cdots, 1$,set

$$y = a_j + y * x_0; \text{(compute } b_j \text{for } P)$$

$$z = y + z * x_0; \text{(compute } c_{j-1} \text{for } Q)$$

Step 3 Set $y = a_0 + y * x_0$,(compute b_0 for P)

Step 5 OUTPUT: $y, (y = P(x_0); z, (z = P'(x_0))$

INPUT
- degree n;
- Coefficients $a_0, a_1, a_2, \cdots, a_n$ of polynomial $P(x)$;
- initial approximation x_0;
- tolerance TOL;
- Maximum iteration number N.

OUTPUT The root p of $P(x) = 0$ or message of failure.

Step 1 Set $i = 1$ and $p_0 = x_0$.

Step 2 while $n \leq N$, do Step 3-8

- **Step 3** Set $y = a_n$(compute b_n for P);
  $z = a_n$(compute c_{n-1} for Q);
- **Step 4** For $j = n-1, n-2, \cdots, 1$,set
  $y = a_j + y * p_0$; (compute b_j for P)
  $z = y + z * p_0$; (compute c_{j-1} for Q)
- **Step 5** Set $y = a_0 + y * p_0$, (compute b_0 for P)
- **Step 6** Compute Newton's approximation

$$p = p_0 - y/z;$$

- **Step 7** If $|p - p_0| < TOL$,output p, STOP.
- **Step 8** Set $i = i + 1, p_0 = p$

Step 9 OUTPUT: (Method failed), STOP.

Remarks:

- Using Newton's method with the help of Horner's method each time, we can get an approximation zero of a polynomial $P(x)$.
- Suppose that if the Nth iteration, x_N, in the Newton-Raphson procedure, is an approximation zero of $P(x)$, then

$$\begin{aligned} P(x) &= (x - x_N)Q(x) + b_0 = (x - x_N)Q(x) + P(x_N) \\ &\approx (x - x_N)Q(x); \end{aligned}$$

- Let $\hat{x}_1 = x_N$ be the approximate zero of P, and $Q_1(x) \equiv Q(x)$ be the approximate factor, then we have

$$P(x) \approx (x - \hat{x}_1)Q_1(x).$$

- To find the second approximate zero of $P(x)$, we can use the same procedure to $Q_1(x)$, give

$$Q_1(x) \approx (x - \hat{x}_2)Q_2(x).$$

where $Q_2(x)$ is a polynomial of degree $n-2$.

- Thus

$$P(x) \approx (x - \hat{x}_1)Q_1(x) \approx (x - \hat{x}_1)(x - \hat{x}_2)Q_2(x).$$

- Repeat this procedure, till $Q_{n-2}(x)$ which is an quadratic polynomial and can be solved by quadratic formula. we can get all approximate zeros of $P(x)$. This method is called **deflation method–压缩技术**
- Theoretically, if $P(x)$ is an nth-degree polynomial with n real zeros, the deflation method can be used to find all approximate zeros. It depends on repeated use of approximations and can lead to very inaccurate results.

- If a polynomial has complex roots, how can we get them by Newton's method?
- One way to solve complex root finding problem during the use of Newton's method is to begin with a complex initial approximation and do all computations using complex arithmetic.

THEOREM 2.19

If $z = a + bi$ is a complex zero of multiplicity m of the polynomial $P(x)$, then

$$\bar{z} = a - bi$$

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 $P(x)$.

- In this part, we consider another method to solve root finding problems especially for **approximating the zeros of polynomials**.
- **Present**: Müller's method is first presented by D.E.Müller in 1956, and can be thought as an extension of the Secant method.
- **Idea:** It uses three initial approximations, x_0, x_1 and x_2, and determines the next approximation x_3 by considering the intersection of the x-axis with the parabola through $(x_0, f(x_0)), (x_1, f(x_1))$ and $(x_2, f(x_2))$.

- It is clear that three point can only determine a quadratic polynomial $P(x)$.
- Suppose that $P(x)$ has the form

$$P(x) = a(x - x_2)^2 + b(x - x_2) + c$$

that passes through $(x_0, f(x_0)), (x_1, f(x_1))$ and $(x_2, f(x_2))$.

- Then we have

$$\begin{cases} f(x_0) = a(x_0 - x_2)^2 + b(x_0 - x_2) + c, \\ f(x_1) = a(x_1 - x_2)^2 + b(x_1 - x_2) + c, \\ f(x_2) = a \times 0 + b \times 0 + c = c, \end{cases}$$

- It is clear that three point can only determine a quadratic polynomial $P(x)$.
- Suppose that $P(x)$ has the form

$$P(x) = a(x - x_2)^2 + b(x - x_2) + c$$

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- Then we have

$$\begin{cases} f(x_0) = a(x_0 - x_2)^2 + b(x_0 - x_2) + c, \\ f(x_1) = a(x_1 - x_2)^2 + b(x_1 - x_2) + c, \\ f(x_2) = a \times 0 + b \times 0 + c = c, \end{cases}$$

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- Suppose that $P(x)$ has the form

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that passes through $(x_0, f(x_0)), (x_1, f(x_1))$ and $(x_2, f(x_2))$.

- Then we have

$$\begin{cases} f(x_0) = a(x_0 - x_2)^2 + b(x_0 - x_2) + c, \\ f(x_1) = a(x_1 - x_2)^2 + b(x_1 - x_2) + c, \\ f(x_2) = a \times 0 + b \times 0 + c = c, \end{cases}$$

- Solve this equations, we can get the coefficients a, b, c of $P(x)$.

$$
\begin{aligned}
c &= f(x_2), \\
a(x_0 - x_2) + b &= \frac{f(x_0) - f(x_2)}{x_0 - x_2}, \\
a(x_1 - x_2) + b &= \frac{f(x_1) - f(x_2)}{x_1 - x_2}.
\end{aligned}
$$

- $\Rightarrow$

$$\begin{aligned}
c &= f(x_2),\\
a &= \frac{\frac{f(x_0)-f(x_2)}{x_0-x_2} - \frac{f(x_1)-f(x_2)}{x_1-x_2}}{x_0 - x_1},\\
&= \frac{\frac{f(x_0)-f(x_1)+f(x_1)-f(x_2)}{x_0-x_2} - \frac{f(x_1)-f(x_2)}{x_1-x_2}}{x_0 - x_1}\\
&= \frac{\frac{f(x_0)-f(x_1)}{x_0-x_2} + (\frac{1}{x_0-x_2} - \frac{1}{x_1-x_2})(f(x_1) - f(x_2))}{x_0 - x_1}\\
&= \frac{\frac{x_0-x_1}{x_0-x_2}\frac{f(x_1)-f(x_0)}{x_1-x_0} + \frac{x_1-x_0}{x_0-x_2}\frac{f(x_2)-f(x_1)}{x_2-x_1}}{x_0 - x_1}\\
&= \frac{\frac{f(x_2)-f(x_1)}{x_2-x_1} - \frac{f(x_1)-f(x_0)}{x_1-x_0}}{x_2 - x_0}\\
b &= \frac{f(x_2) - f(x_1)}{x_2 - x_1} + (x_2 - x_1)a,
\end{aligned}$$

- To determine the intersection x_3 , or a zero of quadratic polynomial $P(x)$,
- we apply the quadratic formula to $P(x) = 0$, and get

$$\begin{aligned} x - x_2 &= \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \\ &= \frac{(-b \pm \sqrt{b^2 - 4ac})(-b \mp \sqrt{b^2 - 4ac})}{2a(-b \mp \sqrt{b^2 - 4ac})}. \end{aligned}$$

- so

$$x - x_2 = \frac{-2c}{b \pm \sqrt{b^2 - 4ac}}$$

- Let $x = x_3$, thus above formula gives two solutions or possibilities for the approximation x_3.
- In Müller's method, the sign is chosen to agree with the sign of b.

$$x_3 = x_2 - \frac{2c}{b + \text{sign}(b)\sqrt{b^2 - 4ac}}$$

- Once x_3 is determined, the procedure is reinitialized using x_1, x_2, x_3 in place of x_0, x_1 and x_2 to determine next approximation x_4.
- The method continues until satisfactory conclusion is obtained.

Müller's Algorithm

To find a solution to $f(x) = 0$ given three approximations x_0, x_1 and x_2.

INPUT x_0, x_1, x_2; tolerance TOL; maximum number of iterations N.

OUTPUT approximate solution p or message of failure.

Step 1 Set

$$\begin{aligned}
h_1 &= x_1 - x_0, h_2 = x_2 - x_1, \\
\delta_1 &= (f(x_1) - f(x_0))/h_1, \\
\delta_2 &= (f(x_2) - f(x_1))/h_2, \\
a &= (\delta_2 - \delta_1)/(h_2 + h_1), \\
i &= 3.
\end{aligned}$$

Step 2 While $i \le N$, do Step 3-7.

Step 3 $b = \delta_2 + h_2 a$, $d = (b^2 - 4 * a * f(x_2))^{1/2}$. (Note: maybe complex arithmetic.)

Step 4 If $|b - d| < |b + d|$, then $e = b + d$, else $e = b - d$.

Step 5 Set $h = -2f(x_2)/e; p = x_2 + h$.

Step 6 If $|h| < TOL$, then OUTPUT p (Procedure completed successfully),STOP.

Step 7 Set (To prepare next iteration)

$$
\begin{aligned}
x_0 &= x_1, x_1 = x_2, x_2 = p; \\
h_1 &= x_1 - x_0, h_2 = x_2 - x_1; \\
\delta_1 &= (f(x_1) - f(x_0))/h_1, \\
\delta_2 &= (f(x_2) - f(x_1))/h_2; \\
a &= (\delta_2 - \delta_1)/(h_2 + h_1), \\
i &= i + 1.
\end{aligned}
$$

Step 8 OUTPUT ('Method failed after N_0 iteration', '$N_0 =$', N_0), STOP.