Solutions of Equations in One Variable

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Outline

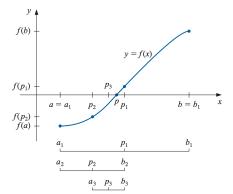
- Bisection Method
- 2 Fixed-Point Iteration
- Newton's method
- Error analysis for iterative methods
- **5** Accelerating convergence
- 6 Zeros of polynomials and Müller's method



Bisection Method

Idea

If $f(x) \in C[a,b]$ and f(a)f(b) < 0, then $\exists \ c \in (a,b)$ such that f(c) = 0.







Bisection method algorithm

End For

Given f(x) defined on (a,b), the maximal number of iterations M, and stop criteria δ and ε , this algorithm tries to locate one root of f(x).

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Compute u=f(a), v=f(b), and e=b-a If sign(u)=sign(v), then stop For k=1,2,\ldots,M e=e/2, c=a+e, w=f(c) If |e|<\delta or |w|<\varepsilon, then stop If sign(w)\neq sign(u) b=c, v=w Else a=c, u=w End If
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Let $\{c_n\}$ be the sequence of numbers produced. The algorithm should stop if one of the following conditions is satisfied.

- the iteration number k > M,
- $|c_k c_{k-1}| < \delta$, or
- $|f(c_k)| < \varepsilon.$

Let $[a_0,b_0],[a_1,b_1],\ldots$ denote the successive intervals produced by the bisection algorithm. Then

$$a=a_0 \leq a_1 \leq a_2 \leq \cdots \leq b_0 = b$$

 $\Rightarrow \{a_n\} \text{ and } \{b_n\} \text{ are bounded}$
 $\Rightarrow \lim_{n \to \infty} a_n \text{ and } \lim_{n \to \infty} b_n \text{ exist}$



Since

$$b_1 - a_1 = \frac{1}{2}(b_0 - a_0)$$

$$b_2 - a_2 = \frac{1}{2}(b_1 - a_1) = \frac{1}{4}(b_0 - a_0)$$

$$\vdots$$

$$b_n - a_n = \frac{1}{2^n}(b_0 - a_0)$$

hence

$$\lim_{n \to \infty} b_n - \lim_{n \to \infty} a_n = \lim_{n \to \infty} (b_n - a_n) = \lim_{n \to \infty} \frac{1}{2^n} (b_0 - a_0) = 0.$$

Therefore

$$\lim_{n \to \infty} a_n = \lim_{n \to \infty} b_n \equiv z.$$

Since *f* is a continuous function, we have that

$$\lim_{n\to\infty} f(a_n) = f(\lim_{n\to\infty} a_n) = f(z) \quad \text{and} \quad \lim_{n\to\infty} f(b_n) = f(\lim_{n\to\infty} b_n) = f(z)$$

On the other hand,

$$f(a_n)f(b_n) < 0$$

$$\Rightarrow \lim_{n \to \infty} f(a_n)f(b_n) = f^2(z) \le 0$$

$$\Rightarrow f(z) = 0$$

Therefore, the limit of the sequences $\{a_n\}$ and $\{b_n\}$ is a zero of f in [a,b]. Let $c_n=\frac{1}{2}(a_n+b_n)$. Then

$$|z - c_n| = \left| \lim_{n \to \infty} a_n - \frac{1}{2} (a_n + b_n) \right|$$

$$= \left| \frac{1}{2} \left[\lim_{n \to \infty} a_n - b_n \right] + \frac{1}{2} \left[\lim_{n \to \infty} a_n - a_n \right] \right|$$

$$\leq \max \left\{ \left| \lim_{n \to \infty} a_n - b_n \right|, \left| \lim_{n \to \infty} a_n - a_n \right| \right\}$$

$$\leq |b_n - a_n| = \frac{1}{2n} |b_0 - a_0|.$$

This proves the following theorem.



Theorem 1

Let $\{[a_n,b_n]\}$ denote the intervals produced by the bisection algorithm. Then $\lim_{n\to\infty} a_n$ and $\lim_{n\to\infty} b_n$ exist, are equal, and represent a zero of f(x). If

$$z = \lim_{n \to \infty} a_n = \lim_{n \to \infty} b_n$$
 and $c_n = \frac{1}{2}(a_n + b_n),$

then

$$|z-c_n| \le \frac{1}{2^n} (b_0 - a_0).$$

Remark

 $\{c_n\}$ converges to z with the rate of $O(2^{-n})$.



Example 2

How many steps should be taken to compute a root of $f(x) = x^3 + 4x^2 - 10 = 0$ on [1,2] with relative error 10^{-3} ?

solution: Seek an n such that

$$\frac{|z - c_n|}{|z|} \le 10^{-3} \implies |z - c_n| \le |z| \times 10^{-3}.$$

Since $z \in [1, 2]$, it is sufficient to show

$$|z - c_n| \le 10^{-3}.$$

That is, we solve

$$2^{-n}(2-1) < 10^{-3} \implies -n \log_{10} 2 < -3$$

which gives n > 10.



Exercise

Page 54: 1, 13, 14, 16, 17



Fixed-Point Iteration

Definition 3

Bisection

x is called a fixed point of a given function g if g(x) = x.

Root-finding problems and fixed-point problems

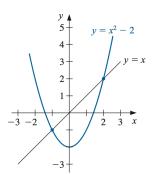
- Find x^* such that $f(x^*) = 0$. Let g(x) = x - f(x). Then $g(x^*) = x^* - f(x^*) = x^*$. $\Rightarrow x^*$ is a fixed point for g(x).
- Find x^* such that $g(x^*) = x^*$. Define f(x) = x - g(x) so that $f(x^*) = x^* - g(x^*) = x^* - x^* = 0$ $\Rightarrow x^*$ is a zero of f(x).

Example 4

Bisection

The function $g(x)=x^2-2$, for $-2 \le x \le 3$, has fixed points at x=-1 and x=2 since

$$0 = g(x) - x = x^2 - x - 2 = (x+1)(x-2).$$

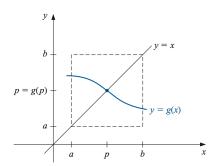






Theorem 5 (Existence and uniqueness)

- If $g \in C[a, b]$ such that $a \leq g(x) \leq b$ for all $x \in [a, b]$, then g has a fixed point in [a, b].
- ② If, in addition, g'(x) exists in (a,b) and there exists a positive constant M < 1 such that $|g'(x)| \le M < 1$ for all $x \in (a,b)$. Then the fixed point is unique.







Proof

Bisection

Existence:

- If g(a) = a or g(b) = b, then a or b is a fixed point of g and we are done.
- Otherwise, it must be g(a) > a and g(b) < b. The function h(x) = g(x) x is continuous on [a,b], with

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

By the Intermediate Value Theorem, $\exists~x^* \in [a,b]$ such that $h(x^*) = 0.$ That is

$$g(x^*) - x^* = 0 \implies g(x^*) = x^*.$$

Hence g has a fixed point x^* in [a, b].



Proof

Uniqueness:

Suppose that $p \neq q$ are both fixed points of g in [a,b]. By the Mean-Value theorem, there exists ξ between p and q such that

$$g'(\xi) = \frac{g(p) - g(q)}{p - q} = \frac{p - q}{p - q} = 1.$$

However, this contradicts to the assumption that $|g'(x)| \leq M < 1$ for all x in [a,b]. Therefore the fixed point of g is unique.



Fixed-Point Iteration

Bisection

$$g(x) = (x^2 - 1)/3, \quad x \in [-1, 1].$$

Solution: The Extreme Value Theorem implies that

$$\min_{x \in [-1,1]} g(x) = g(0) = -\frac{1}{3},$$

$$\max_{x \in [-1,1]} g(x) = g(\pm 1) = 0.$$

That is $g(x) \in [-1,1], \ \forall \ x \in [-1,1].$ Moreover, g is continuous and

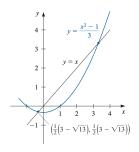
$$|g'(x)| = \left|\frac{2x}{3}\right| \le \frac{2}{3}, \ \forall \ x \in (-1, 1).$$

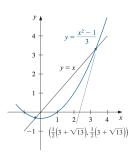
By above theorem, g has a unique fixed point in [-1, 1].

Let p be such unique fixed point of g. Then

$$p = g(p) = \frac{p^2 - 1}{3} \Rightarrow p^2 - 3p - 1 = 0$$

 $\Rightarrow p = \frac{1}{2}(3 - \sqrt{13}).$









Fixed-point iteration or functional iteration

Given a continuous function g, choose an initial point x_0 and generate $\{x_k\}_{k=0}^{\infty}$ by

$$x_{k+1} = g(x_k), \quad k \ge 0.$$

 $\{x_k\}$ may not converge, e.g., g(x)=3x. However, when the sequence converges, say,

$$\lim_{k \to \infty} x_k = x^*,$$

then, since g is continuous,

Bisection

$$g(x^*) = g(\lim_{k \to \infty} x_k) = \lim_{k \to \infty} g(x_k) = \lim_{k \to \infty} x_{k+1} = x^*.$$

That is, x^* is a fixed point of g.



Fixed-point iteration

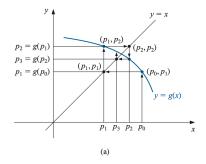
Given x_0 , tolerance TOL, maximum number of iteration M.

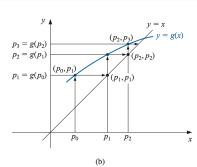
Set
$$i = 1$$
 and $x = g(x_0)$.

While $i \leq M$ and $|x - x_0| \geq TOL$

Set i = i + 1, $x_0 = x$ and $x = g(x_0)$.

End While







Example 7

Bisection

The equation

$$x^3 + 4x^2 - 10 = 0$$

has a unique root in [1,2]. Change the equation to the fixed-point form x=g(x).

(a)
$$x = g_1(x) \equiv x - f(x) = x - x^3 - 4x^2 + 10$$

(b)
$$x = g_2(x) = \left(\frac{10}{x} - 4x\right)^{1/2}$$

$$x^{3} = 10 - 4x^{2} \implies x^{2} = \frac{10}{x} - 4x \implies x = \pm \left(\frac{10}{x} - 4x\right)^{1/2}$$



Zeros of polynomials

(c)
$$x = g_3(x) = \frac{1}{2} (10 - x^3)^{1/2}$$

$$4x^2 = 10 - x^3 \quad \Rightarrow \quad x = \pm \frac{1}{2} \left(10 - x^3\right)^{1/2}$$

(d)
$$x = g_4(x) = \left(\frac{10}{4+x}\right)^{1/2}$$

$$x^{2}(x+4) = 10 \implies x = \pm \left(\frac{10}{4+x}\right)^{1/2}$$

(e)
$$x = g_5(x) = x - \frac{x^3 + 4x^2 - 10}{3x^2 + 8x}$$

$$x = g_5(x) \equiv x - \frac{f(x)}{f'(x)}$$



Results of the fixed-point iteration with initial point $x_0=1.5$

n	(a)	(b)	(c)	(<i>d</i>)	(e)
0	1.5	1.5	1.5	1.5	1.5
1	-0.875	0.8165	1.286953768	1.348399725	1.373333333
2	6.732	2.9969	1.402540804	1.367376372	1.365262015
3	-469.7	$(-8.65)^{1/2}$	1.345458374	1.364957015	1.365230014
4	1.03×10^{8}		1.375170253	1.365264748	1.365230013
5			1.360094193	1.365225594	
6			1.367846968	1.365230576	
7			1.363887004	1.365229942	
8			1.365916734	1.365230022	
9			1.364878217	1.365230012	
10			1.365410062	1.365230014	
15			1.365223680	1.365230013	
20			1.365230236		
25			1.365230006		
30			1.365230013		

Theorem 8 (Fixed-point Theorem)

Bisection

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

$$|g'(x)| \le k, \ \forall \ x \in (a,b).$$

Then, for any number x_0 in [a, b],

$$x_n = g(x_{n-1}), \ n \ge 1,$$

converges to the unique fixed point x in [a,b].



Proof: By the assumptions, a unique fixed point exists in [a,b]. Since $g([a,b])\subseteq [a,b],$ $\{x_n\}_{n=0}^{\infty}$ is defined and $x_n\in [a,b]$ for all $n\geq 0$. Using the Mean Values Theorem and the fact that $|g'(x)|\leq k$, we have

$$|x - x_n| = |g(x_{n-1}) - g(x)| = |g'(\xi_n)||x - x_{n-1}| \le k|x - x_{n-1}|,$$

where $\xi_n \in (a, b)$. It follows that

$$|x_n - x| \le k|x_{n-1} - x| \le k^2|x_{n-2} - x| \le \dots \le k^n|x_0 - x|.$$
 (1)

Since 0 < k < 1, we have

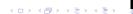
$$\lim_{n \to \infty} k^n = 0$$

and

Bisection

$$\lim_{n \to \infty} |x_n - x| \le \lim_{n \to \infty} k^n |x_0 - x| = 0.$$

Hence, $\{x_n\}_{n=0}^{\infty}$ converges to x.



Corollary 9

If q satisfies the hypotheses of above theorem, then

$$|x - x_n| \le k^n \max\{x_0 - a, b - x_0\}$$

and

$$|x_n - x| \le \frac{k^n}{1 - k} |x_1 - x_0|, \ \forall \ n \ge 1.$$

Proof: From (1),

$$|x_n - x| \le k^n |x_0 - x| \le k^n \max\{x_0 - a, b - x_0\}.$$

For $n \geq 1$, using the Mean Values Theorem,

$$|x_{n+1} - x_n| = |g(x_n) - g(x_{n-1})| \le k|x_n - x_{n-1}| \le \dots \le k^n|x_1 - x_0|$$

Thus, for $m > n \ge 1$,

Bisection

$$|x_{m} - x_{n}| = |x_{m} - x_{m-1} + x_{m-1} - \dots + x_{n+1} - x_{n}|$$

$$\leq |x_{m} - x_{m-1}| + |x_{m-1} - x_{m-2}| + \dots + |x_{n+1} - x_{n}|$$

$$\leq k^{m-1}|x_{1} - x_{0}| + k^{m-2}|x_{1} - x_{0}| + \dots + k^{n}|x_{1} - x_{0}|$$

$$= k^{n}|x_{1} - x_{0}| \left(1 + k + k^{2} + \dots + k^{m-n-1}\right).$$

It implies that

$$|x - x_n| = \lim_{m \to \infty} |x_m - x_n| \le \lim_{m \to \infty} k^n |x_1 - x_0| \sum_{j=0}^{m-n-1} k^j$$

$$\le k^n |x_1 - x_0| \sum_{j=0}^{\infty} k^j = \frac{k^n}{1 - k} |x_1 - x_0|.$$



Example 10

Bisection

For previous example,

$$f(x) = x^3 + 4x^2 - 10 = 0.$$

For $q_1(x) = x - x^3 - 4x^2 + 10$, we have

$$g_1(1) = 6$$
 and $g_1(2) = -12$,

so $g_1([1,2]) \nsubseteq [1,2]$. Moreover,

$$g_1'(x) = 1 - 3x^2 - 8x \quad \Rightarrow \quad |g_1'(x)| \ge 1 \ \forall \ x \in [1, 2]$$

DOES NOT guarantee to converge or not

For
$$g_3(x) = \frac{1}{2}(10 - x^3)^{1/2}, \ \forall \ x \in [1, 1.5],$$

$$g_3'(x) = -\frac{3}{4}x^2(10 - x^3)^{-1/2} < 0, \ \forall \ x \in [1, 1.5],$$

so g_3 is strictly decreasing on [1, 1.5] and

$$1 < 1.28 \approx g_3(1.5) \le g_3(x) \le g_3(1) = 1.5, \ \forall \ x \in [1, 1.5].$$

On the other hand,

$$|g_3'(x)| \le |g_3'(1.5)| \approx 0.66, \ \forall \ x \in [1, 1.5].$$

Hence, the sequence is convergent to the fixed point.

$$\sqrt{\frac{10}{6}} \le g_4(x) \le \sqrt{\frac{10}{5}}, \ \forall \ x \in [1, 2] \quad \Rightarrow \quad g_4([1, 2]) \subseteq [1, 2]$$

Moreover,

$$|g_4'(x)| = \left| \frac{-5}{\sqrt{10}(4+x)^{3/2}} \right| \le \frac{5}{\sqrt{10}(5)^{3/2}} < 0.15, \ \forall \ x \in [1, 2].$$

The bound of $|g'_4(x)|$ is much smaller than the bound of $|g'_3(x)|$, which explains the more rapid convergence using g_4 .



Exercise

Page 64: 1, 3, 7, 11, 13



Suppose that $f:\mathbb{R}\to\mathbb{R}$ and $f\in C^2[a,b]$, i.e., f'' exists and is continuous. If $f(x^*)=0$ and $x^*=x+h$ where h is small, then by Taylor's theorem

$$0 = f(x^*) = f(x+h)$$

$$= f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{3!}f'''(x)h^3 + \cdots$$

$$= f(x) + f'(x)h + O(h^2).$$

Since ${\it h}$ is small, $O(h^2)$ is negligible. It is reasonable to drop $O(h^2)$ terms. This implies

$$f(x) + f'(x)h \approx 0$$
 and $h \approx -\frac{f(x)}{f'(x)}$, if $f'(x) \neq 0$.

Hence

$$x + h = x - \frac{f(x)}{f'(x)}$$

is a better approximation to x^* .



This sets the stage for the Newton-Rapbson's method, which starts with an initial approximation x_0 and generates the sequence $\{x_n\}_{n=0}^{\infty}$ defined by

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}.$$

Since the Taylor's expansion of f(x) at x_n is given by

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

At x_n , one uses the tangent line

$$y = \ell(x) = f(x_n) + f'(x_n)(x - x_n)$$

to approximate the curve of f(x) and uses the zero of the tangent line to approximate the zero of f(x).



Newton's Method

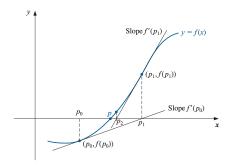
Given x_0 , tolerance TOL, maximum number of iteration M.

Set
$$n = 1$$
 and $x = x_0 - f(x_0)/f'(x_0)$.

While
$$n \leq M$$
 and $|x - x_0| \geq TOL$

Set
$$n = n + 1$$
, $x_0 = x$ and $x = x_0 - f(x_0)/f'(x_0)$.

End While







Three stopping-technique inequalities

(a).
$$|x_n - x_{n-1}| < \varepsilon$$
,

(b).
$$\frac{|x_n - x_{n-1}|}{|x_n|} < \varepsilon, \quad x_n \neq 0,$$

(c).
$$|f(x_n)| < \varepsilon$$
.

Note that Newton's method for solving f(x) = 0

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \text{ for } n \ge 1$$

is just a special case of functional iteration in which

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

Example 11

Bisection

The following table shows the convergence behavior of Newton's method applied to solving $f(x)=x^2-1=0$. Observe the quadratic convergence rate.

n	x_n	$ e_n \equiv 1 - x_n $
0	2.0	1
1	1.25	0.25
2	1.025	2.5e-2
3	1.0003048780488	3.048780488e-4
4	1.0000000464611	4.64611e-8
5	1.0	0





Theorem 12

Bisection

Assume $f(x^*) = 0$, $f'(x^*) \neq 0$ and f(x), f'(x) and f''(x) are continuous on $N_{\varepsilon}(x^*)$. Then if x_0 is chosen sufficiently close to x^* , then

$$\left\{ x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \right\} \to x^*.$$

Proof: Define

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

Find an interval $[x^* - \delta, x^* + \delta]$ such that

$$g([x^* - \delta, x^* + \delta]) \subseteq [x^* - \delta, x^* + \delta]$$

and

$$|q'(x)| \le k < 1, \ \forall \ x \in (x^* - \delta, x^* + \delta).$$



Since f' is continuous and $f'(x^*) \neq 0$, it implies that $\exists \ \delta_1 > 0$ such that $f'(x) \neq 0 \ \forall \ x \in [x^* - \delta_1, x^* + \delta_1] \subseteq [a, b]$. Thus, g is defined and continuous on $[x^* - \delta_1, x^* + \delta_1]$. Also

Bisection

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

for $x\in[x^*-\delta_1,x^*+\delta_1]$. Since f'' is continuous on [a,b], we have g' is continuous on $[x^*-\delta_1,x^*+\delta_1]$. By assumption $f(x^*)=0$, so

$$g'(x^*) = \frac{f(x^*)f''(x^*)}{|f'(x^*)|^2} = 0.$$

Since g' is continuous on $[x^*-\delta_1,x^*+\delta_1]$ and $g'(x^*)=0$, $\exists \ \delta$ with $0<\delta<\delta_1$ and $k\in(0,1)$ such that

$$|g'(x)| \le k, \ \forall \ x \in [x^* - \delta, x^* + \delta].$$



Claim: $q([x^* - \delta, x^* + \delta]) \subset [x^* - \delta, x^* + \delta]$. If $x \in [x^* - \delta, x^* + \delta]$, then, by the Mean Value Theorem, $\exists \xi$ between x and x^* such that

$$|g(x) - g(x^*)| = |g'(\xi)||x - x^*|.$$

It implies that

$$|g(x) - x^*| = |g(x) - g(x^*)| = |g'(\xi)||x - x^*|$$

$$\leq k|x - x^*| < |x - x^*| < \delta.$$

Hence, $g([x^* - \delta, x^* + \delta]) \subseteq [x^* - \delta, x^* + \delta]$.

By the Fixed-Point Theorem, the sequence $\{x_n\}_{n=0}^{\infty}$ defined by

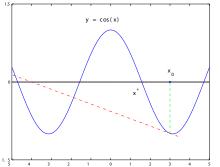
$$x_n = g(x_{n-1}) = x_{n-1} - \frac{f(x_{n-1})}{f'(x_{n-1})}, \text{ for } n \ge 1,$$

converges to x^* for any $x_0 \in [x^* - \delta, x^* + \delta]$.



Example 13

When Newton's method applied to $f(x)=\cos x$ with starting point $x_0=3$, which is close to the root $\frac{\pi}{2}$ of f, it produces $x_1=-4.01525, x_2=-4.8526, \cdots$, which converges to another root $-\frac{3\pi}{2}$.







Secant method

Bisection

Disadvantage of Newton's method

In many applications, the derivative f'(x) is very expensive to compute, or the function f(x) is not given in an algebraic formula so that f'(x) is not available.

By definition,

$$f'(x_{n-1}) = \lim_{x \to x_{n-1}} \frac{f(x) - f(x_{n-1})}{x - x_{n-1}}.$$

If x_{n-2} is close to x_{n-1} , then

$$f'(x_{n-1}) \approx \frac{f(x_{n-2}) - f(x_{n-1})}{x_{n-2} - x_{n-1}} = \frac{f(x_{n-1}) - f(x_{n-2})}{x_{n-1} - x_{n-2}}.$$

Using this approximation for $f'(x_{n-1})$ in Newton's formula gives

$$x_n = x_{n-1} - \frac{f(x_{n-1})(x_{n-1} - x_{n-2})}{f(x_{n-1}) - f(x_{n-2})},$$

From geometric point of view, we use a secant line through x_{n-1} and x_{n-2} instead of the tangent line to approximate the function at the point x_{n-1} .

The slope of the secant line is

$$s_{n-1} = \frac{f(x_{n-1}) - f(x_{n-2})}{x_{n-1} - x_{n-2}}$$

and the equation is

$$M(x) = f(x_{n-1}) + s_{n-1}(x - x_{n-1}).$$

The zero of the secant line

$$x = x_{n-1} - \frac{f(x_{n-1})}{s_{n-1}} = x_{n-1} - f(x_{n-1}) \frac{x_{n-1} - x_{n-2}}{f(x_{n-1}) - f(x_{n-2})}$$

is then used as a new approximate x_n .



Secant Method

Bisection

Given x_0, x_1 , tolerance TOL, maximum number of iteration M.

Set
$$i = 2$$
; $y_0 = f(x_0)$; $y_1 = f(x_1)$;

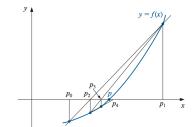
$$x = x_1 - y_1(x_1 - x_0)/(y_1 - y_0).$$

While $i \leq M$ and $|x - x_1| \geq TOL$

Set
$$i = i + 1$$
; $x_0 = x_1$; $y_0 = y_1$; $x_1 = x$; $y_1 = f(x)$;

$$x = x_1 - y_1(x_1 - x_0)/(y_1 - y_0).$$

End While







Method of False Position

- Choose initial approximations x_0 and x_1 with $f(x_0)f(x_1) < 0$.
- 2 $x_2 = x_1 f(x_1)(x_1 x_0)/(f(x_1) f(x_0))$
- Oecide which secant line to use to compute x_3 : If $f(x_2)f(x_1) < 0$, then x_1 and x_2 bracket a root, i.e.,

$$x_3 = x_2 - f(x_2)(x_2 - x_1)/(f(x_2) - f(x_1))$$

Else, x_0 and x_2 bracket a root, i.e.,

$$x_3 = x_2 - f(x_2)(x_2 - x_0)/(f(x_2) - f(x_0))$$

End if



Method of False Position

Given x_0, x_1 , tolerance TOL, maximum number of iteration M.

Set
$$i = 2$$
; $y_0 = f(x_0)$; $y_1 = f(x_1)$; $x = x_1 - y_1(x_1 - x_0)/(y_1 - y_0)$.

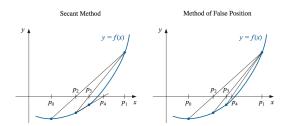
While $i \leq M$ and $|x - x_1| \geq TOL$

Set
$$i = i + 1$$
; $y = f(x)$.

If
$$y \cdot y_1 < 0$$
, then set $x_0 = x_1; y_0 = y_1$.

Set
$$x_1 = x$$
; $y_1 = y$; $x = x_1 - y_1(x_1 - x_0)/(y_1 - y_0)$.

End While







Exercise

Page 75: 12, 17, 18



Error analysis for iterative methods

Definition 14

Let $\{x_n\} \to x^*$. If there are positive constants c and α such that

$$\lim_{n \to \infty} \frac{|x_{n+1} - x^*|}{|x_n - x^*|^{\alpha}} = c,$$

then $\{x_n\}$ converges to x^* of order α with asymptotic error constant c.

- **1** linear convergence if $\alpha = 1$ and 0 < c < 1.
- 2 superlinear convergence if

$$\lim_{n \to \infty} \frac{|x_{n+1} - x^*|}{|x_n - x^*|} = 0;$$

3 quadratic convergence if $\alpha = 2$.

Suppose that $\{x_n\}_{n=0}^{\infty}$ and $\{\tilde{x}_n\}_{n=0}^{\infty}$ are linearly and quadratically convergent to x^* , respectively, with the same constant c=0.5. For simplicity, suppose that

$$\frac{|x_{n+1}-x^*|}{|x_n-x^*|}\approx c\quad\text{and}\quad\frac{|\tilde{x}_{n+1}-x^*|}{|\tilde{x}_n-x^*|^2}\approx c.$$

These imply that

$$|x_n - x^*| \approx c|x_{n-1} - x^*| \approx c^2|x_{n-2} - x^*| \approx \cdots \approx c^n|x_0 - x^*|,$$

and

Bisection

$$|\tilde{x}_n - x^*| \approx c|\tilde{x}_{n-1} - x^*|^2 \approx c \left[c|\tilde{x}_{n-2} - x^*|^2\right]^2 = c^3 |\tilde{x}_{n-2} - x^*|^4$$

$$\approx c^3 \left[c|\tilde{x}_{n-3} - x^*|^2\right]^4 = c^7 |\tilde{x}_{n-3} - x^*|^8$$

$$\approx \cdots \approx c^{2^n - 1} |\tilde{x}_0 - x^*|^{2^n}.$$



Remark

Quadratically convergent sequences generally converge much more quickly thank those that converge only linearly.

Theorem 15

Let $g \in C[a,b]$ with $g([a,b]) \subseteq [a,b]$. Suppose that g' is continuous on (a,b) and $\exists \ k \in (0,1)$ such that

$$|g'(x)| \le k, \ \forall \ x \in (a, b).$$

If $g'(x^*) \neq 0$, then for any $x_0 \in [a, b]$, the sequence

$$x_n = g(x_{n-1}), \text{ for } n \ge 1$$

converges only linearly to the unique fixed point x^* in [a, b].

Proof:

- By the Fixed-Point Theorem, the sequence $\{x_n\}_{n=0}^{\infty}$ converges to x^* .
- Since g' exists on (a,b), by the Mean Value Theorem, $\exists \ \xi_n$ between x_n and x^* such that

$$x_{n+1} - x^* = g(x_n) - g(x^*) = g'(\xi_n)(x_n - x^*).$$

- $\bullet :: \{x_n\}_{n=0}^{\infty} \to x^* \quad \Rightarrow \quad \{\xi_n\}_{n=0}^{\infty} \to x^*$
- Since g' is continuous on (a, b), we have

$$\lim_{n \to \infty} g'(\xi_n) = g'(x^*).$$

Thus,

$$\lim_{n \to \infty} \frac{|x_{n+1} - x^*|}{|x_n - x^*|} = \lim_{n \to \infty} |g'(\xi_n)| = |g'(x^*)|.$$

Hence, if $g'(x^*) \neq 0$, fixed-point iteration exhibits linear convergence.



Theorem 16

Let x^* be a fixed point of g and I be an open interval with $x^* \in I$. Suppose that $g'(x^*) = 0$ and g'' is continuous with

$$|g''(x)| < M, \ \forall \ x \in I.$$

Then $\exists \ \delta > 0$ such that

$$\{x_n = g(x_{n-1})\}_{n=1}^{\infty} \to x^* \text{ for } x_0 \in [x^* - \delta, x^* + \delta]$$

at least quadratically. Moreover,

$$|x_{n+1}-x^*|<\frac{M}{2}|x_n-x^*|^2$$
, for sufficiently large n .

Proof:

• Since $g'(x^*)=0$ and g' is continuous on I, $\exists \ \delta$ such that $[x^*-\delta,x^*+\delta]\subset I$ and

$$|g'(x)| \le k < 1, \ \forall \ x \in [x^* - \delta, x^* + \delta].$$

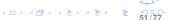
 In the proof of the convergence for Newton's method, we have

$$\{x_n\}_{n=0}^{\infty} \subset [x^* - \delta, x^* + \delta].$$

• Consider the Taylor expansion of $g(x_n)$ at x^*

$$x_{n+1} = g(x_n) = g(x^*) + g'(x^*)(x_n - x^*) + \frac{g''(\xi_n)}{2}(x_n - x^*)^2$$
$$= x^* + \frac{g''(\xi_n)}{2}(x_n - x^*)^2,$$

where ξ_n lies between x_n and x^* .



Since

$$|g'(x)| \le k < 1, \ \forall \ x \in [x^* - \delta, x^* + \delta]$$

and

$$g([x^* - \delta, x^* + \delta]) \subseteq [x^* - \delta, x^* + \delta],$$

it follows that $\{x_n\}_{n=0}^{\infty}$ converges to x^* .

• But ξ_n is between x_n and x^* for each n, so $\{\xi_n\}_{n=0}^\infty$ also converges to x^* and

$$\lim_{n \to \infty} \frac{|x_{n+1} - x^*|}{|x_n - x^*|^2} = \frac{|g''(x^*)|}{2} < \frac{M}{2}.$$

• It implies that $\{x_n\}_{n=0}^{\infty}$ is quadratically convergent to x^* if $g''(x^*) \neq 0$ and

$$|x_{n+1}-x^*|<\frac{M}{2}|x_n-x^*|^2$$
, for sufficiently large n .



For Newton's method,

Bisection

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

It follows that $g'(x^*) = 0$. Hence Newton's method is locally quadratically convergent.



Bisection

Multiple Roots

Definition 17

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

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

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

Theorem 18

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

$$0 = f(p) = f'(p) = f''(p) = \dots = f^{(m-1)}(p),$$

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

Define

Bisection

$$\mu(x) = \frac{f(x)}{f'(x)}.$$

If p is a zero of f of multiplicity m with

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

then

$$\mu(x) = \frac{(x-p)^m q(x)}{m(x-p)^{m-1} q(x) + (x-p)^m q'(x)}$$
$$= (x-p) \frac{q(x)}{mq(x) + (x-p)q'(x)}.$$

Since $q(p) \neq 0$ and

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

p is a simple root of $\mu(x)$.

Newton's method can be applied to $\mu(x)$ to give

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

- Linear convergence of Newton's method for f(x).
- ② Quadratic convergence of Newton's method for $\mu(x)$.
- 3 Multiple roots can cause serious round-off problems because $[f'(x)]^2 f(x)f''(x)$ consists of the difference of two numbers that are both close to 0.



Error Analysis of Secant Method

Bisection

Reference: D. Kincaid and W. Cheney, "Numerical analysis" Let x^* denote the exact solution of f(x) = 0, $e_n = x_n - x^*$ be the error at the n-th step. Then

$$e_{n+1} = x_{n+1} - x^*$$

$$= x_n - f(x_n) \frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} - x^*$$

$$= \frac{1}{f(x_n) - f(x_{n-1})} [(x_{n-1} - x^*) f(x_n) - (x_n - x^*) f(x_{n-1})]$$

$$= \frac{1}{f(x_n) - f(x_{n-1})} (e_{n-1} f(x_n) - e_n f(x_{n-1}))$$

$$= e_n e_{n-1} \left(\frac{\frac{1}{e_n} f(x_n) - \frac{1}{e_{n-1}} f(x_{n-1})}{x_n - x_{n-1}} \cdot \frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} \right)$$

$$f(x_n) = f(x^* + e_n) = f(x^*) + f'(x^*)e_n + \frac{1}{2}f''(x^*)e_n^2 + O(e_n^3),$$

to get

$$\frac{1}{e_n}f(x_n) = f'(x^*) + \frac{1}{2}f''(x^*)e_n + O(e_n^2).$$

Similarly,

$$\frac{1}{e_{n-1}}f(x_{n-1}) = f'(x^*) + \frac{1}{2}f''(x^*)e_{n-1} + O(e_{n-1}^2).$$

Hence

$$\frac{1}{e_n}f(x_n) - \frac{1}{e_{n-1}}f(x_{n-1}) \approx \frac{1}{2}(e_n - e_{n-1})f''(x^*).$$

Since $x_n - x_{n-1} = e_n - e_{n-1}$ and

$$\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} \to \frac{1}{f'(x^*)},$$

we have

$$e_{n+1} \approx e_n e_{n-1} \left(\frac{\frac{1}{2} (e_n - e_{n-1}) f''(x^*)}{e_n - e_{n-1}} \cdot \frac{1}{f'(x^*)} \right) = \frac{1}{2} \frac{f''(x^*)}{f'(x^*)} e_n e_{n-1}$$

$$\equiv C e_n e_{n-1}. \tag{2}$$

To estimate the convergence rate, we assume

$$|e_{n+1}| \approx \eta |e_n|^{\alpha},$$

where $\eta > 0$ and $\alpha > 0$ are constants, i.e.,

$$rac{|e_{n+1}|}{\eta|e_n|^{lpha}}
ightarrow 1 \quad {
m as} \quad n
ightarrow \infty.$$

Then $|e_n| \approx \eta |e_{n-1}|^{\alpha}$ which implies $|e_{n-1}| \approx \eta^{-1/\alpha} |e_n|^{1/\alpha}$. Hence (2) gives

$$\eta |e_n|^{\alpha} \approx C|e_n|\eta^{-1/\alpha}|e_n|^{1/\alpha} \quad \Longrightarrow \quad C^{-1}\eta^{1+\frac{1}{\alpha}} \approx |e_n|^{1-\alpha+\frac{1}{\alpha}}.$$

Since $|e_n| \to 0$ as $n \to \infty$, and $C^{-1}\eta^{1+\frac{1}{\alpha}}$ is a nonzero constant,

$$1 - \alpha + \frac{1}{\alpha} = 0 \implies \alpha = \frac{1 + \sqrt{5}}{2} \approx 1.62.$$

This result implies that $C^{-1}\eta^{1+\frac{1}{\alpha}} \to 1$ and

$$\eta \to C^{\frac{\alpha}{1+\alpha}} = \left(\frac{f''(x^*)}{2f'(x^*)}\right)^{0.62}.$$

In summary, we have shown that

$$|e_{k+1}| = \eta |e_k|^{\alpha}, \quad \alpha \approx 1.62,$$

that is, the convergence of Secant method is superlinear.

Order of convergence

- secant method: superlinear
- Newton's method: quadratic
- bisection method: linear

Each iteration of method requires

- secant method: one function evaluation
- Newton's method: two function evaluation, namely, $f(x_n)$ and $f'(x_n)$.
- \Rightarrow two steps of secant method are comparable to one step of Newton's method. Thus

$$|e_{n+2}| \approx \eta |e_{n+1}|^{\alpha} \approx \eta^{1+\alpha} |e_n|^{\frac{3+\sqrt{5}}{2}} \approx \eta^{1+\alpha} |e_n|^{2.62}.$$

⇒ secant method is more efficient than Newton's method.

Remark

Two steps of secant method would require a little more work than one step of Newton's method.

Exercise

Page 85: 8, 9, 10, 11





Aitken's Δ^2 method

- Accelerate the convergence of a sequence that is linearly convergent.
- Suppose $\{y_n\}_{n=0}^{\infty}$ is a linearly convergent sequence with limit y. Construct a sequence $\{\hat{y}_n\}_{n=0}^{\infty}$ that converges more rapidly to y than $\{y_n\}_{n=0}^{\infty}$.

For *n* sufficiently large,

$$\frac{y_{n+1} - y}{y_n - y} \approx \frac{y_{n+2} - y}{y_{n+1} - y}.$$

Then

$$(y_{n+1} - y)^2 \approx (y_{n+2} - y)(y_n - y),$$

SO

$$y_{n+1}^2 - 2y_{n+1}y + y^2 \approx y_{n+2}y_n - (y_{n+2} + y_n)y + y^2$$



Bisection

$$(y_{n+2} + y_n - 2y_{n+1})y \approx y_{n+2}y_n - y_{n+1}^2$$
.

Solving for y gives

$$y \approx \frac{y_{n+2}y_n - y_{n+1}^2}{y_{n+2} - 2y_{n+1} + y_n}$$

$$= \frac{y_n y_{n+2} - 2y_n y_{n+1} + y_n^2 - y_n^2 + 2y_n y_{n+1} - y_{n+1}^2}{y_{n+2} - 2y_{n+1} + y_n}$$

$$= \frac{y_n (y_{n+2} - 2y_{n+1} + y_n) - (y_{n+1} - y_n)^2}{(y_{n+2} - y_{n+1}) - (y_{n+1} - y_n)}$$

$$= y_n - \frac{(y_{n+1} - y_n)^2}{(y_{n+2} - y_{n+1}) - (y_{n+1} - y_n)}.$$

Aitken's Δ^2 method

$$\hat{y}_n = y_n - \frac{(y_{n+1} - y_n)^2}{(y_{n+2} - y_{n+1}) - (y_{n+1} - y_n)}.$$
 (3)

Zeros of polynomials

Example 19

Bisection

The sequence $\{y_n = \cos(1/n)\}_{n=1}^{\infty}$ converges linearly to y = 1.

\overline{n}	y_n	\hat{y}_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	

• $\{\hat{y}_n\}_{n=1}^{\infty}$ converges more rapidly to y=1 than $\{y_n\}_{n=1}^{\infty}$.



Definition 20

For a given sequence $\{y_n\}_{n=0}^{\infty}$, the forward difference Δy_n is defined by

$$\Delta y_n = y_{n+1} - y_n$$
, for $n \ge 0$.

Higher powers of Δ are defined recursively by

$$\Delta^k y_n = \Delta(\Delta^{k-1} y_n), \quad \text{for } k \ge 2.$$

The definition implies that

$$\Delta^2 y_n = \Delta (y_{n+1} - y_n) = \Delta y_{n+1} - \Delta y_n = (y_{n+2} - y_{n+1}) - (y_{n+1} - y_n).$$

So the formula for \hat{y}_n in (3) can be written as

$$\hat{y}_n = y_n - \frac{(\Delta y_n)^2}{\Delta^2 y_n}, \quad \text{for } n \ge 0.$$



Theorem 21

Suppose $\{y_n\}_{n=0}^{\infty} \to y$ linearly and

$$\lim_{n \to \infty} \frac{y_{n+1} - y}{y_n - y} < 1.$$

Then $\{\hat{y}_n\}_{n=0}^{\infty} \to y$ faster than $\{y_n\}_{n=0}^{\infty}$ in the sense that

$$\lim_{n \to \infty} \frac{\hat{y}_n - y}{y_n - y} = 0.$$

• Aitken's Δ^2 method constructs the terms in order:

$$y_0, \quad y_1 = g(y_0), \quad y_2 = g(y_1), \quad \hat{y}_0 = \{\Delta^2\}(y_0), \quad y_3 = g(y_2),$$

 $\hat{y}_1 = \{\Delta^2\}(y_1), \quad \dots$

$$\Rightarrow$$
 Assume $|\hat{y}_0 - y| < |y_2 - y|$



Bisection

Steffensen's method constructs the terms in order:

$$y_0^{(0)} \equiv y_0,$$
 $y_1^{(0)} = g(y_0^{(0)}),$ $y_2^{(0)} = g(y_1^{(0)}),$ $y_0^{(1)} = \{\Delta^2\}(y_0^{(0)}),$ $y_1^{(1)} = g(y_0^{(1)}),$ $y_2^{(1)} = g(y_1^{(1)}),$

Steffensen's method (To find a solution of y = g(y))

Given y_0 , tolerance Tol, max. number of iteration M. Set i = 1.

While
$$i \leq M$$

Set $y_1 = g(y_0)$; $y_2 = g(y_1)$; $y = y_0 - (y_1 - y_0)^2/(y_2 - 2y_1 + y_0)$.

If
$$|y-y_0| < Tol$$
, then STOP.

Set
$$i = i + 1$$
; $y_0 = y$.

End While

Theorem 22

Suppose x=g(x) has solution x^* with $g'(x^*) \neq 1$. If $\exists \ \delta > 0$ such that $g \in C^3[x^*-\delta,x^*+\delta]$, then Steffensen's method gives quadratic convergence for any $x_0 \in [x^*-\delta,x^*+\delta]$.

Exercise

Page 90: 4, 5, 8, 13





Horner's method:

Let

$$P(x) = a_0 + a_1 x + a_2 x^2 + \dots + a_{n-1} x^{n-1} + a_n x^n$$

= $a_0 + x (a_1 + x (a_2 + \dots + x (a_{n-1} + a_n x) \dots)).$

lf

$$b_n = a_n,$$

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

then

$$b_0 = a_0 + b_1 x_0 = a_0 + (a_1 + b_2 x_0) x_0 = \dots = P(x_0).$$

Consider

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



Then

$$b_0 + (x - x_0)Q(x) = b_0 + (x - x_0) (b_1 + b_2 x + \dots + b_n x^{n-1})$$

$$= (b_0 - b_1 x_0) + (b_1 - b_2 x_0)x + \dots + (b_{n-1} - b_n x_0)x^{n-1} + b_n x^n$$

$$= a_0 + a_1 x + \dots + a_n x^n = P(x).$$

Differentiating P(x) with respect to x gives

$$P'(x) = Q(x) + (x - x_0)Q'(x)$$
 and $P'(x_0) = Q(x_0)$.

Use Newton-Raphson method to find an approximate zero of P(x):

$$x_{k+1} = x_k - \frac{P(x_k)}{Q(x_k)}, \ \forall \ k = 0, 1, 2, \dots$$

Similarly, let

$$c_n = b_n = a_n,$$

 $c_k = b_k + c_{k+1}x_k, \text{ for } k = n-1, n-2, \dots, 1,$

then $c_1 = Q(x_k)$.



Horner's method (Evaluate $y = P(x_0)$ and $z = P'(x_0)$)

Set
$$y = a_n$$
; $z = a_n$.
For $j = n - 1, n - 2, ..., 1$
Set $y = a_j + yx_0$; $z = y + zx_0$.
End for
Set $y = a_0 + yx_0$.

If x_N is an approximate zero of P, then

$$P(x) = (x - x_N)Q(x) + b_0 = (x - x_N)Q(x) + P(x_N)$$

 $\approx (x - x_N)Q(x) \equiv (x - \hat{x}_1)Q_1(x).$

So $x-\hat{x}_1$ is an approximate factor of P(x) and we can find a second approximate zero of P by applying Newton's method to $Q_1(x)$. The procedure is called deflation.

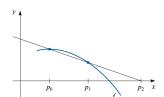
• Müller's method for complex root:

Theorem 23

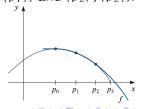
Bisection

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

Secant method: Given p_0 and p_1 , determine p_2 as the intersection of the x-axis with the line through $(p_0, f(p_0))$ and $(p_1, f(p_1))$.



Müller's method: Given p_0, p_1 and p_2 , determine p_3 by the intersection of the x-axis with the parabola through $(p_0, f(p_0))$, $(p_1, f(p_1))$ and $(p_2, f(p_2))$.





Let

$$P(x) = a(x - p_2)^2 + b(x - p_2) + c$$

that passes through $(p_0,f(p_0))$, $(p_1,f(p_1))$ and $(p_2,f(p_2))$. Then

$$f(p_0) = a(p_0 - p_2)^2 + b(p_0 - p_2) + c,$$

$$f(p_1) = a(p_1 - p_2)^2 + b(p_1 - p_2) + c,$$

$$f(p_2) = a(p_2 - p_2)^2 + b(p_2 - p_2) + c = c.$$

It implies that

$$c = f(p_2),$$

$$b = \frac{(p_0 - p_2)^2 [f(p_1) - f(p_2)] - (p_1 - p_2)^2 [f(p_0) - f(p_2)]}{(p_0 - p_2)(p_1 - p_2)(p_0 - p_1)}$$

$$a = \frac{(p_1 - p_2) [f(p_0) - f(p_2)] - (p_0 - p_2) [f(p_1) - f(p_2)]}{(p_0 - p_2)(p_1 - p_2)(p_0 - p_1)}.$$

To determine p_3 , a zero of P, we apply the quadratic formula to P(x)=0 and get

$$p_3 - p_2 = \frac{2c}{b \pm \sqrt{b^2 - 4ac}}.$$

Choose

$$p_3 = p_2 + \frac{2c}{b + sqn(b)\sqrt{b^2 - 4ac}}$$

such that the denominator will be largest and result in p_3 selected as the closest zero of P to p_2 .



Müller's method (Find a solution of f(x) = 0)

Given p_0, p_1, p_2 ; tolerance TOL; maximum number of iterations M

Set
$$h_1 = p_1 - p_0$$
; $h_2 = p_2 - p_1$;
 $\delta_1 = (f(p_1) - f(p_0))/h_1$; $\delta_2 = (f(p_2) - f(p_1))/h_2$;
 $d = (\delta_2 - \delta_1)/(h_2 + h_1)$; $i = 3$.

While $i \leq M$

Bisection

Set
$$b = \delta_2 + h_2 d$$
; $D = \sqrt{b^2 - 4f(p_2)d}$.

If
$$|b-D| < |b+D|$$
, then set $E = b+D$ else set $E = b-D$.

Set
$$h = -2f(p_2)/E$$
; $p = p_2 + h$.

If
$$|h| < TOL$$
, then STOP.

Set
$$p_0 = p_1$$
; $p_1 = p_2$; $p_2 = p$; $h_1 = p_1 - p_0$; $h_2 = p_2 - p_1$; $\delta_1 = (f(p_1) - f(p_0))/h_1$; $\delta_2 = (f(p_2) - f(p_1))/h_2$; $d = (\delta_2 - \delta_1)/(h_2 + h_1)$; $i = i + 1$.

End while



Exercise

Page 100: 9

