Numerical Analysis I
Solutions of Equations in One Variable

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[1] These slides are based on Prof. Tsung-Ming Huang(NTNU)'s original slides

Outline

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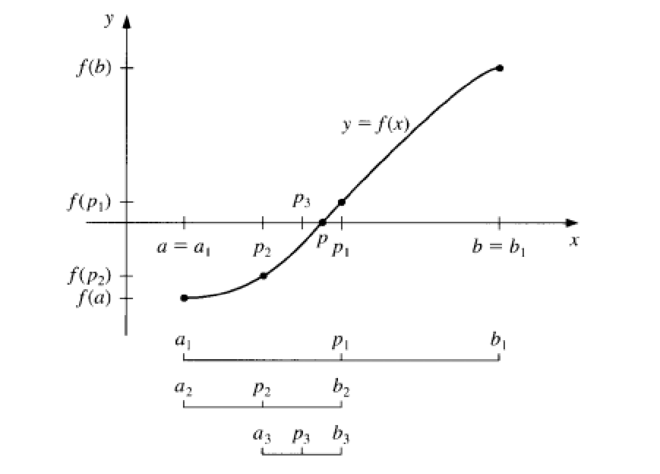
Bisection Method

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

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 $f(x)$.

Compute $fa = f(a)$, $fb = f(b)$, and $e = b - a$
If $sign(fa) = sign(fb)$, **then** stop **End If**
For $k = 1, 2, \cdots, M$
  $e = e/2$, $c = (a + b)/2$, $fc = f(c)$
  If $(|e| < \delta$ or $|fc| < \varepsilon)$, **then** stop **End If**
  If $sign(fc) \neq sign(fa)$
    $b = c$, $fb = fc$
  Else
    $a = c$, $fa = fc$
  End If
End For

Let $\{c_n\}$ be the sequence of numbers produced. The algorithm should stop if one of the following conditions is satisfied.

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

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

$$\begin{aligned} & a = a_0 \le a_1 \le a_2 \le \cdots \le b_0 = b \\ \Rightarrow \quad & \{a_n\} \text{ and } \{b_n\} \text{ are bounded} \\ \Rightarrow \quad & \lim_{n\to\infty} a_n \text{ and } \lim_{n\to\infty} b_n \text{ exist} \end{aligned}$$

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Since

$$
\begin{aligned}
b_1 - a_1 &= \frac{1}{2}(b_0 - a_0) \\
b_2 - a_2 &= \frac{1}{2}(b_1 - a_1) = \frac{1}{4}(b_0 - a_0) \\
&\vdots \\
b_n - a_n &= \frac{1}{2^n}(b_0 - a_0)
\end{aligned}
$$

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,

$$
\begin{aligned}
& f(a_n)f(b_n) < 0 \\
\Rightarrow \quad & \lim_{n\to\infty} f(a_n)f(b_n) = f^2(z) \le 0 \\
\Rightarrow \quad & f(z) = 0
\end{aligned}
$$

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

$$
\begin{aligned}
|z - c_n| &= \left|\lim_{n\to\infty} a_n - \frac{1}{2}(a_n + b_n)\right| \\
&= \left|\frac{1}{2}\left[\lim_{n\to\infty} a_n - b_n\right] + \frac{1}{2}\left[\lim_{n\to\infty} a_n - a_n\right]\right| \\
&\le \max\left\{\left|\lim_{n\to\infty} a_n - b_n\right|, \left|\lim_{n\to\infty} a_n - a_n\right|\right\} \\
&\le |b_n - a_n| = \frac{1}{2^n}|b_0 - a_0|.
\end{aligned}
$$

This proves the following theorem.

Theorem

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*

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

then

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

Remark

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

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Example

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

$$\frac{|z - c_n|}{|z|} \leq 10^{-3} \;\Rightarrow\; |z - c_n| \leq |z| \times 10^{-3}.$$

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

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

That is, we solve

$$2^{-n}(2 - 1) \leq 10^{-3} \;\Rightarrow\; -n \log_{10} 2 \leq -3$$

which gives $n \geq 10$.

Fixed-Point Iteration

Definition

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

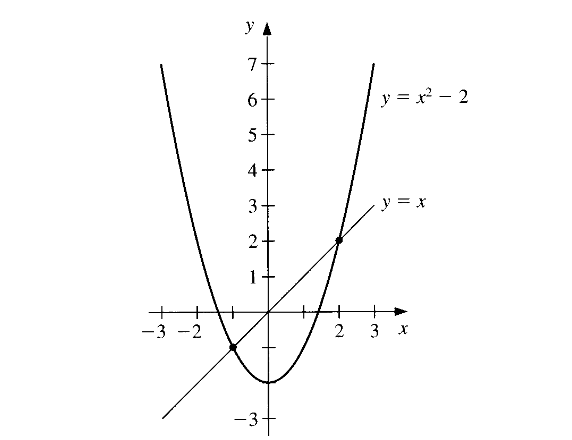
Root-finding problems and fixed-point problems

- 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

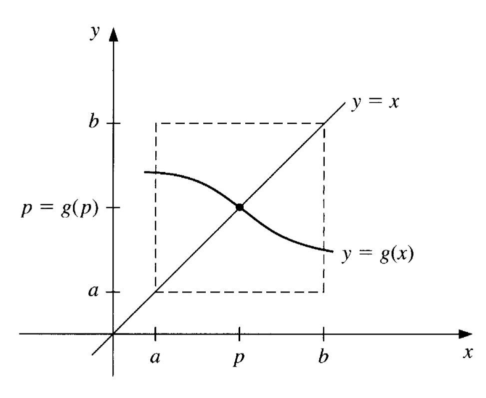
The function $g(x) = x^2 - 2$, for $-2 \leq x \leq 3$, has fixed points at $x = -1$ and $x = 2$ since

$$g(-1) = (-1)^2 - 2 = -1 \quad \text{and} \quad g(2) = 2^2 - 2 = 2.$$



Theorem (Existence and uniqueness)

1. *If* $g \in C[a, b]$ *such that* $a \le g(x) \le b$ *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

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

  $$h(a) = g(a) - a > 0 \text{ and } h(b) = g(b) - b < 0.$$

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

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

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

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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. $\square$

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Example

Show that the following function has a unique fixed point.

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

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

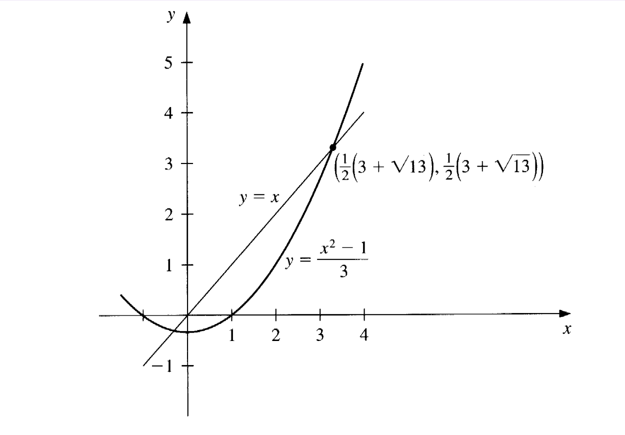
$$|g'(x)| = \left|\frac{2x}{3}\right| \leq \frac{2}{3}, \ \forall\, x \in (-1, 1).$$

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

Let p be such unique fixed point of g. Then

$$p = g(p) = \frac{p^2 - 1}{3} \quad \Rightarrow \quad p^2 - 3p - 1 = 0$$
$$\Rightarrow \quad p = \frac{1}{2}(3 - \sqrt{13}).$$

□



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

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

$\{x_k\}$ 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,

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

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

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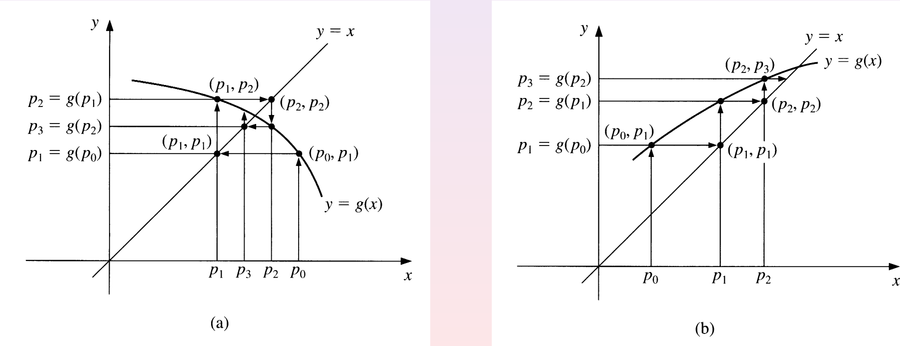
Fixed-point iteration

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

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

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

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

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

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

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

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

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

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

n	(a)	(b)	(c)	(d)	(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		

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Theorem (Fixed-point Theorem)

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 with $0 < k < 1$ such that

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

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

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

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

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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

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

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

$$|x_n - x| \leq k|x_{n-1} - x| \leq k^2|x_{n-2} - x| \leq \cdots \leq k^n|x_0 - x|. \tag{1}$$

Since $0 < k < 1$, we have

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

and

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

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

Corollary

If g satisfies the hypotheses of above theorem, then

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

and

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

Proof: From (1),

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

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

$$|x_{n+1} - x_n| = |g(x_n) - g(x_{n-1})| \leq k|x_n - x_{n-1}| \leq \cdots \leq k^n |x_1 - x_0|.$$

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

$$\begin{aligned} |x_m - x_n| &= |x_m - x_{m-1} + x_{m-1} - \cdots + x_{n+1} - x_n| \\ &\leq |x_m - x_{m-1}| + |x_{m-1} - x_{m-2}| + \cdots + |x_{n+1} - x_n| \\ &\leq k^{m-1}|x_1 - x_0| + k^{m-2}|x_1 - x_0| + \cdots + k^n|x_1 - x_0| \\ &= k^n|x_1 - x_0| \left(1 + k + k^2 + \cdots + k^{m-n-1}\right). \end{aligned}$$

It implies that

$$\begin{aligned} |x - x_n| &= \lim_{m\to\infty} |x_m - x_n| \leq \lim_{m\to\infty} k^n|x_1 - x_0| \sum_{j=0}^{m-n-1} k^j \\ &\leq k^n|x_1 - x_0| \sum_{j=0}^{\infty} k^j = \frac{k^n}{1-k}|x_1 - x_0|. \end{aligned}$$

Example

For previous example, $f(x) = x^3 + 4x^2 - 10 = 0$.

Let $g_1(x) = x - x^3 - 4x^2 + 10$, we have

$$g_1(1) = 6 \quad \text{and} \quad g_1(2) = -12,$$

so $g_1([1,2]) \not\subseteq [1,2]$. Moreover,

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

Convergence is NOT guaranteed. In fact, it almost for sure will not converge since when x_n is close to the solution x^*,

$$|x_n - x^*| = |g_1(x_{n-1}) - g_1(x^*)| = |g_1'(c)(x_{n-1} - x^*)| > |x_{n-1} - x^*|.$$

The error is amplified whenever x_n is close to convergence. The only possibility for convergence is when x_n is far from x^* and (by chance, and very unlikely) that $g_1(x_n) = x^*$.

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.

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For $g_4(x) = \sqrt{10/(4+x)}$, we have

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

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.

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Generalized (Modified) Fixed-Point Iteration

If the fixed-point iteration

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

diverges or converges slowly, one can modify it to

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

by choosing suitable α (fixed) or α_k (k-dependent) to accelerate the convergence.

Since

$$e_{k+1} = \alpha e_k + (1-\alpha) g'(\xi_k) e_k = \left(\alpha + (1-\alpha) g'(\xi_k)\right) e_k$$

It follows that the optimal α is given by

$$\alpha + (1-\alpha) g'(\xi_k) \approx 0$$

Possible choice of α or α_k include:

- $\alpha_k + (1-\alpha_k) g'(x_k) = 0$,
- or $\alpha + (1-\alpha) g'(\frac{a+b}{2}) = 0$ or $\alpha + (1-\alpha)\frac{g(b)-g(a)}{b-a} = 0$.

Newton's method

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

$$\begin{aligned} 0 = f(x^*) &= f(x+h) \\ &= f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{3!}f'''(x)h^3 + \cdots \\ &= f(x) + f'(x)h + O(h^2). \end{aligned}$$

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

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

Hence

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

is a better approximation to x^*.

This sets the stage for the Newton-Raphson'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_k is given by

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

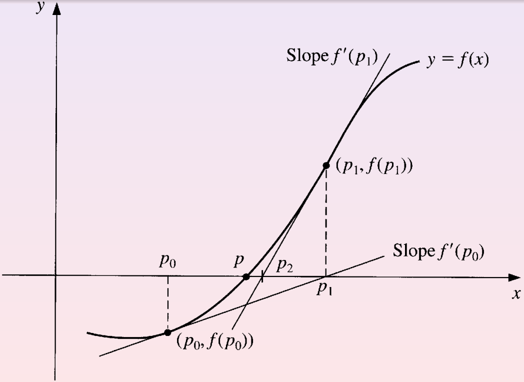
At x_k, one uses the tangent line

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

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 $i = 1$ and $x = x_0 - f(x_0)/f'(x_0)$.
While $i \leq M$ and $|x - x_0| \geq TOL$
  Set $i = i + 1$, $x_0 = x$ and $x = x_0 - f(x_0)/f'(x_0)$.
End While



Three stopping-technique inequalities

$$
\begin{aligned}
&(a). \quad |x_n - x_{n-1}| < \varepsilon, \\
&(b). \quad \frac{|x_n - x_{n-1}|}{|x_n|} < \varepsilon, \quad x_n \neq 0, \\
&(c). \quad |f(x_n)| < \varepsilon.
\end{aligned}
$$

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

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

is just a special case of functional iteration in which

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

Example

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

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Theorem

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

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

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

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

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

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

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

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

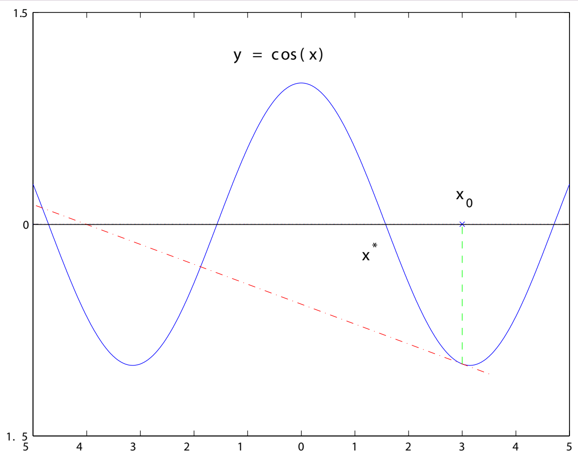
Hence, $g([x^* - \delta, x^* + \delta]) \subseteq [x^* - \delta, x^* + \delta]$.
By the Fixed-Point Theorem, the sequence $\{x_n\}_{n=0}^{\infty}$ defined by

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

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

Example

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

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,

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

Letting $x = x_{n-2}$, we have

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

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

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

which is called the Secant method.

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.

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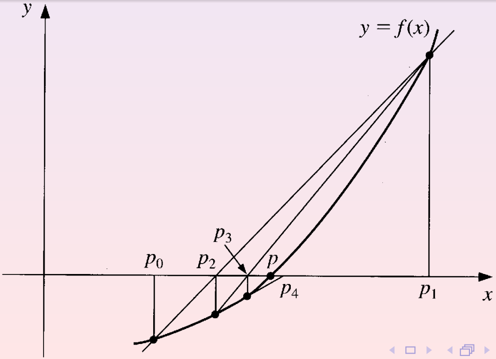
Secant Method

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 $i \le M$ and $|x - x_1| \ge TOL$
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

1. Choose initial approximations x_0 and x_1 with $f(x_0)f(x_1) < 0$.
2. $x_2 = x_1 - f(x_1)(x_1 - x_0)/(f(x_1) - f(x_0))$
3. Decide 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

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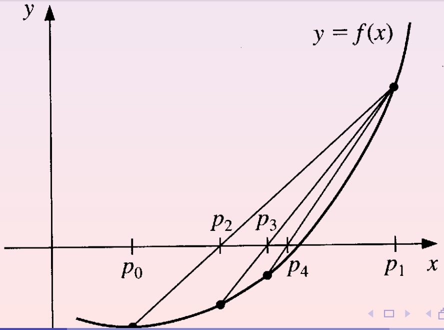
Method of False Position

Given p_0, p_1, tolerance TOL, maximum number of iteration M.
Set $i = 2$; $q_{\text{older}} = q_0$); $q_{\text{old}} = q_1$; $q_0 = f(p_0)$; $q_1 = f(p_1)$;
While $i \leq M$ and $|p - p_1| \geq TOL$
    $p = p_1 - q_1(p_1 - p_0)/(q_1 - q_0)$.
    Set $i = i + 1$; $q = f(p)$.
    If $q \cdot q_1 < 0$, then set $p_0 = p_1$; $q_0 = q_1$.
    Set $p_1 = p$; $q_1 = q$;
End While



Error analysis for iterative methods

Definition

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 we say the rate of convergence is of order α.

We say that the rate of convergence is

1. linear if $\alpha = 1$ and $0 < c < 1$.
2. superlinear if
$$\lim_{n\to\infty} \frac{|x_{n+1} - x^*|}{|x_n - x^*|} = 0;$$
3. quadratic 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

$$\begin{aligned} |\tilde{x}_n - x^*| &\approx c|\tilde{x}_{n-1} - x^*|^2 \approx c\left[c|\tilde{x}_{n-2} - x^*|^2\right]^2 = c^3|\tilde{x}_{n-2} - x^*|^4 \\ &\approx c^3\left[c|\tilde{x}_{n-3} - x^*|^2\right]^4 = c^7|\tilde{x}_{n-3} - x^*|^8 \\ &\approx \cdots \approx c^{2^n-1}|\tilde{x}_0 - x^*|^{2^n}. \end{aligned}$$

Remark

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

Theorem

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*

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

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

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

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

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

- $\because \{x_n\}_{n=0}^{\infty} \to x^* \quad \Rightarrow \quad \{\xi_n\}_{n=0}^{\infty} \to x^*$
- 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

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*

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

at least quadratically. Moreover,

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

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Proof:

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

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

- 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^*

$$\begin{aligned} x_{n+1} = g(x_n) &= g(x^*) + g'(x^*)(x_n - x^*) + \frac{g''(\xi)}{2}(x_n - x^*)^2 \\ &= x^* + \frac{g''(\xi)}{2}(x_n - x^*)^2, \end{aligned}$$

where ξ lies between x_n and x^*.

- Since
$$|g'(x)| \leq k < 1, \ \forall \ x \in [x^* - \delta, x^* + \delta]$$
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
$$|x_{n+1} - x^*| < \frac{M}{2}|x_n - x^*|^2, \quad \text{for sufficiently large} \quad n. \qquad \square$$

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Example

Recall that Newton's method $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$ corresponds to $g(x) = x - \frac{f(x)}{f'(x)}$. Suppose that $f(x)$ has a m-fold root at x^*, that is

$$f(x) = (x - x^*)^m q(x), \qquad q(x^*) \neq 0.$$

Let $\mu(x) = \frac{f(x)}{f'(x)} = (x - x^*)\frac{q(x)}{mq(x)+(x-x^*)q'(x)}$, it is easy to see that $\mu'(x^*) = \frac{1}{m}$. It follows that $0 \leq g'(x_*) = 1 - \frac{1}{m} < 1$. Hence Newton's method is locally convergent. Moreover, it converges quadratically for simple roots ($m = 1$) and linearly for multiple roots ($m > 1$).

Remedy for slow convergence on multiple roots ($m > 1$):

- If m is known, take $x_{n+1} = x_n - \frac{mf(x_n)}{f'(x_n)}$.
- If m is not known, take $x_{n+1} = x_n - \frac{\mu(x_n)}{\mu'(x_n)}$, since $\mu(x) = \frac{f(x)}{f'(x)} = \frac{O(x-x^*)^m}{O(x-x^*)^{m-1}} = O(x - x^*)$ always has a simple root at x^* for any $m \geq 1$. This is known as modified Newton's method.

Global Convergence for Convex (Concave) Functions

Theorem

If $f \in C^2$, $f'' > 0$ and $f(x) = 0$ has a root, then Newton's method always converges to a root x^* for any initial x_0.

Proof:

It suffices to consider the case where $f' > 0$, $f'' > 0$ and $f(x) = 0$ has a root. In this case, the root x^* is unique. Define $e_n = x_n - x^*$. Since $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$. It follows that

$$e_{n+1} = e_n - \frac{f(x_n)}{f'(x_n)}. \tag{2}$$

Moreover, since $f(x^*) = f(x_n) + f'(x_n)(x^* - x_n) + \frac{f''(\xi_n)}{2}(x^* - x_n)^2$, we also have $f(x_n) = f'(x_n)e_n - \frac{f''(\xi_n)}{2}e_n^2$. Therefore

$$e_{n+1} = e_n - \frac{f(x_n)}{f'(x_n)} = \frac{f''(\xi_n)}{2f'(x_n)}e_n^2 > 0. \tag{3}$$

Consequently $x_{n+1} > x^*$ and $f(x_{n+1}) > 0$ for all $n \geq 0$.

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Moreover $e_{n+1} = e_n - \frac{f(x_n)}{f'(x_n)} < e_n$, we conclude that

$$0 < \ldots < x_{n+1} < x_n < \ldots < x_1$$

and x_n converges monotonically to some $\tilde{x}$ satisfying $\tilde{x} = \tilde{x} - \frac{f(\tilde{x})}{f'(\tilde{x})}$, that is $f(\tilde{x}) = 0$, thus $\tilde{x} = x^*$ by uniqueness of the root.

The proof for other cases

- $f' < 0$, $f'' > 0$, $f(x) = 0$ has a root.
- $f'' > 0$, has two distinct roots.
- $f'' > 0$, has a double root.

are similar. So is the concave case ($f'' < 0$).

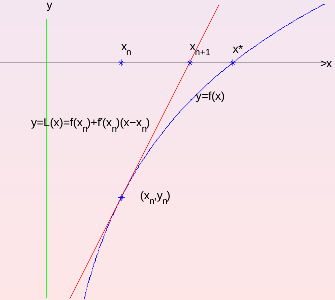
Alternative Error Estimate for Newton's Method

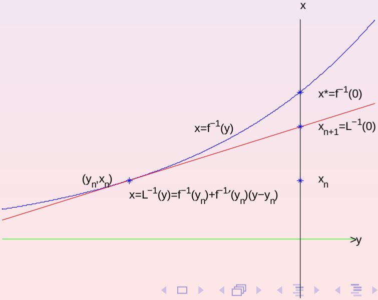
Suppose $f'(x^*) \neq 0$, then both $f(x)$ and its linearization at (x_n, y_n), $L_n(x)$, are locally invertible (Inverse Function Theorem). The formula of the tangent lines are given by

$$L_n(x) = f(x_n) + \frac{df(x_n)}{dx}(x - x_n)$$

and

$$L_n^{-1}(y) = f^{-1}(y_n) + \frac{df^{-1}(y_n)}{dy}(y - y_n) = x_n + \frac{1}{f'(x_n)}(y - y_n)$$





Since $x^* = f^{-1}(0)$ and $x_{n+1} = L_n^{-1}(0)$, the error estimate for Newton's method reduces to error estimate between $f^{-1}(y)$ and its linearization approximation $L_n^{-1}(y)$ at $y = 0$. From standard analysis, the error is proportional to $(0 - y_n)^2$:

$$|x_{n+1} - x^*| = |L_n^{-1}(0) - f^{-1}(0)| = \frac{1}{2}\left|\frac{d^2 f^{-1}}{dy^2}(\eta_n)(y_n - 0)^2\right|$$

$$= \frac{1}{2}\left|\frac{d^2 f^{-1}}{dy^2}(\eta_n)\right| \left(f(x_n) - f(x^*)\right)^2 = \left(\frac{1}{2}\left|\frac{d^2 f^{-1}}{dy^2}(\eta_n)\right| \cdot \left(f'(\xi_n)\right)^2\right)(x_n - x^*)^2$$

The main advantage of this formulation:
Higher order approximations of $f^{-1}(0)$, such as quadratic approximation, gives rise to higher order iteration schemes for solving the original equation $f(x) = 0$.

Error Analysis of Secant Method

Reference: D. Kincaid and W. Cheney, "Numerical analysis"

Let x^* denote the exact solution of $f(x) = 0$, $e_k = x_k - x^*$ be the errors at the k-th step. Then

$$
\begin{aligned}
e_{k+1} &= x_{k+1} - x^* \\
&= x_k - f(x_k)\frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})} - x^* \\
&= \frac{1}{f(x_k) - f(x_{k-1})}\left[(x_{k-1} - x^*)f(x_k) - (x_k - x^*)f(x_{k-1})\right] \\
&= \frac{1}{f(x_k) - f(x_{k-1})}\left(e_{k-1}f(x_k) - e_k f(x_{k-1})\right) \\
&= e_k e_{k-1}\left(\frac{\frac{1}{e_k}f(x_k) - \frac{1}{e_{k-1}}f(x_{k-1})}{x_k - x_{k-1}} \cdot \frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})}\right)
\end{aligned}
$$

To estimate the numerator $\frac{\frac{1}{e_k}f(x_k)-\frac{1}{e_{k-1}}f(x_{k-1})}{x_k-x_{k-1}}$, we apply the Taylor's theorem

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

to get

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

Similarly,

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

Hence

$$\frac{1}{e_k}f(x_k) - \frac{1}{e_{k-1}}f(x_{k-1}) \approx \frac{1}{2}(e_k - e_{k-1})f''(x^*).$$

Since $x_k - x_{k-1} = e_k - e_{k-1}$ and

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

we have

$$\begin{aligned} e_{k+1} &\approx e_k e_{k-1}\left(\frac{\frac{1}{2}(e_k-e_{k-1})f''(x^*)}{e_k-e_{k-1}}\cdot\frac{1}{f'(x^*)}\right)=\frac{1}{2}\frac{f''(x^*)}{f'(x^*)}e_k e_{k-1} \\ &\equiv Ce_k e_{k-1} \end{aligned} \quad (4)$$

To estimate the convergence rate, we assume

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

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

$$\frac{|e_{k+1}|}{\eta|e_k|^{\alpha}}\to 1 \quad \text{as} \quad k\to\infty.$$

Then $|e_k|\approx \eta|e_{k-1}|^{\alpha}$ which implies $|e_{k-1}|\approx \eta^{-1/\alpha}|e_k|^{1/\alpha}$. Hence (4) gives

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

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

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

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 rate of convergence is superlinear.
Rate of convergence:

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

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Each iteration of method requires

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

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

  $\Rightarrow$ 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.

Accelerating convergence

Aitken's Δ^2 method

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

For n sufficiently large,

$$\frac{x_{n+1}-x}{x_n-x} \approx \frac{x_{n+2}-x}{x_{n+1}-x}.$$

Then

$$(x_{n+1}-x)^2 \approx (x_{n+2}-x)(x_n-x),$$

so

$$x_{n+1}^2 - 2x_{n+1}x + x^2 \approx x_{n+2}x_n - (x_{n+2}+x_n)x + x^2$$

and

$$(x_{n+2} + x_n - 2x_{n+1})x \approx x_{n+2}x_n - x_{n+1}^2.$$

Solving for x gives

$$\begin{aligned}
x &\approx \frac{x_{n+2}x_n - x_{n+1}^2}{x_{n+2} - 2x_{n+1} + x_n} \\
&= \frac{x_n x_{n+2} - 2x_n x_{n+1} + x_n^2 - x_n^2 + 2x_n x_{n+1} - x_{n+1}^2}{x_{n+2} - 2x_{n+1} + x_n} \\
&= \frac{x_n(x_{n+2} - 2x_{n+1} + x_n) - (x_{n+1} - x_n)^2}{(x_{n+2} - x_{n+1}) - (x_{n+1} - x_n)} \\
&= x_n - \frac{(x_{n+1} - x_n)^2}{(x_{n+2} - x_{n+1}) - (x_{n+1} - x_n)}.
\end{aligned}$$

Aitken's Δ^2 method

$$\hat{x}_n = x_n - \frac{(x_{n+1} - x_n)^2}{(x_{n+2} - x_{n+1}) - (x_{n+1} - x_n)} := \{\Delta^2\}x_n. \tag{5}$$

Theorem

Suppose $\{x_n\}_{n=0}^{\infty} \to x$ *linearly and*

$$\lim_{n\to\infty} \frac{x_{n+1}-x}{x_n - x} < 1.$$

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

$$\lim_{n\to\infty} \frac{\hat{x}_n - x}{x_n - x} = 0.$$

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

$$\begin{aligned} &x_1 = g(x_0), \quad x_2 = g(x_1), \quad &&\hat{x}_0 = \{\Delta^2\}(x_0), \quad x_3 = g(x_2), \\ &\hat{x}_1 = \{\Delta^2\}(x_1), \quad &&\hat{x}_2 = \{\Delta^2\}(x_2), \quad \cdots, \end{aligned}$$

This is based on the assumption that $|\hat{x}_0 - x| < |x_2 - x|$, $|\hat{x}_1 - x| < |x_3 - x|$, etc.

Example

The sequence $\{x_n = \cos(\frac{1}{n})\}_{n=1}^{\infty}$ converges linearly to $x = 1$.

n	x_n	e_n	$\hat{x}_n$	$\hat{e}_n$
1	0.54030	0.45969	0.96178	0.03822
2	0.87758	0.12242	0.98213	0.01787
3	0.94496	0.05504	0.98979	0.01021
4	0.96891	0.03109	0.99342	0.00658
5	0.98007	0.01993	0.99541	0.00459
6	0.98614	0.01386		
7	0.98981	0.01019		

- Note that $\lim_{n\to\infty} \frac{x_{n+1}-x}{x_n-x} = 1$. The assumption in previous Theorem is not satisfied. In this case, $\{\hat{x}_n\}_{n=1}^{\infty}$ converges more rapidly to $x = 1$ than $\{x_{n+2}\}_{n=1}^{\infty}$, but is of the same order. In fact $\hat{e}_n/e_{n+2} \sim 1/3$ for large n. (Why?)

- Steffensen's method constructs the terms in order:

$$
\begin{aligned}
&x_0^{(0)} = x_0, && x_1^{(0)}(= x_1) = g(x_0^{(0)}), && x_2^{(0)}(= x_2) = g(x_1^{(0)}),\\
&x_0^{(1)}(= x_3) = \{\Delta^2\}(x_0^{(0)}), && x_1^{(1)}(= x_4) = g(x_0^{(1)}), && x_2^{(1)}(= x_5) = g(x_1^{(1)}),\\
&x_0^{(2)}(= x_6) = \{\Delta^2\}(x_0^{(1)}), && x_1^{(2)}(= x_7) = g(x_0^{(2)}), && x_2^{(2)}(= x_8) = g(x_1^{(2)}),\\
&\quad \cdots,
\end{aligned}
$$

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

Given x_0, tolerance TOL, maximum number of iteration M.
Set $i = 1$.
While $i \leq M$
  Set $x_1 = g(x_0)$; $x_2 = g(x_1)$; $x = x_0 - (x_1 - x_0)^2/(x_2 - 2x_1 + x_0)$.
  If $|x - x_0| < Tol$, then STOP.
  Set $i = i + 1$; $x_0 = x$.
End While

Theorem

Suppose that $x = g(x)$ has the 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 $x_0 \in [x^* - \delta, x^* + \delta]$.

Proof:

We denote by x_0, x_1, x_2, $\cdots$, (instead of $x_0^{(i)}$, $x_1^{(i)}$, $x_2^{(i)}$), the sequence generated by Steffensen's method.

We will show that $|x_3 - x| \leq C|x_0 - x|^2$, $|x_6 - x| \leq C|x_3 - x|^2$, etc. to establish quadratic convergence. Denote by $\Delta_i = x_i - x^*$, we have

$$\begin{aligned}
\Delta_1 = x_1 - x^* &= g(x_0) - g(x^*) \\
&= g'(x^*)(x_0 - x^*) + \frac{g''(x^*)}{2}(x_0 - x^*)^2 + O(\Delta_0^3) \\
\Delta_2 = x_2 - x^* &= g(x_1) - g(x^*) \\
&= g'(x^*)(x_1 - x^*) + \frac{g''(x^*)}{2}(x_1 - x^*)^2 + O(\Delta_1^3) \\
&= g'(x^*)^2\Delta_0 + \left(\frac{g'(x^*)g''(x^*)}{2} + \frac{g''(x^*)g'(x^*)^2}{2}\right)\Delta_0^2 + O(\Delta_0^3)
\end{aligned}$$

$$
\begin{aligned}
x_3 &= x_0 - \frac{(x_1 - x_0)^2}{x_0 - 2x_1 + x_2} \\
\Delta_3 &= \Delta_0 - \frac{(\Delta_1 - \Delta_0)^2}{\Delta_0 - 2\Delta_1 + \Delta_2} \\
&= \Delta_0 - \frac{\left((g'(x) - 1)\Delta_0 + \frac{g''(x)}{2}\Delta_0^2 + O(\Delta_0^3)\right)^2}{(g'^2(x) - 2g'(x) + 1)\Delta_0 + \frac{g''(x)}{2}(g'^2(x) + g'(x) - 2)\Delta_0^2 + O(\Delta_0^3)} \\
&= \Delta_0 - \Delta_0 \left(\frac{(g'(x) - 1)^2 + g''(x)(g'(x) - 1)\Delta_0 + O(\Delta_0^2)}{(g'(x) - 1)^2 + \frac{g''(x)}{2}(g'(x) + 2)(g'(x) - 1)\Delta_0 + O(\Delta_0^2)} \right) \\
&= \Delta_0 - \Delta_0 \left(1 - \frac{g'(x^*)g''(x^*)}{2(g'(x^*) - 1)}\Delta_0 + O(\Delta_0^2) \right), \quad \text{if } g'(x^*) \neq 1
\end{aligned}
$$

It follows that $x_3 - x \approx C(x_0 - x)^2$, $x_6 - x \approx C(x_3 - x)^2$, etc. with $C = \frac{g'(x^*)g''(x^*)}{2(g'(x^*)-1)}$ if $g'(x^*) \neq 1$.

Zeros of polynomials and Müller's method

• Horner's method:

Goal: Find successively all roots of a polynomial

$$P(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_{n-1} x^{n-1} + a_n x^n \tag{6}$$

with minimal computational cost.

The key step is to efficiently compute the quotient $P(x)/(x - x^*)$ when a root x^* of $P(x)$ has been found (eg. by Newton's method), or more generally, to find the quotient $Q(x)$ and the remainder b_0 such that

$$P(x) = (x - x_k)Q(x) + b_0, \tag{7}$$

for any given x_k. As a byproduct, one obtains $P'(x_k) = Q(x_k)$ from (7) which can be utilized in the Newton-Raphson iteration $x_{k+1} = x_k - \frac{P(x_k)}{P'(x_k)}$.

The coefficients of $Q(x)$ can be obtained by assuming

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

and then comparing the coefficients in (6) and (7).

We have

$$\begin{aligned} & b_0 + (x - x_k)Q(x) = b_0 + (x - x_k)\left(b_1 + b_2 x + \cdots + b_n x^{n-1}\right) \\ = & (b_0 - b_1 x_k) + (b_1 - b_2 x_k)x + \cdots + (b_{n-1} - b_n x_k)x^{n-1} + b_n x^n \\ = & a_0 + a_1 x + \cdots + a_n x^n = P(x). \end{aligned}$$

and therefore

$$\begin{aligned} b_n &= a_n, \\ b_j &= a_j + b_{j+1}x_k, \quad \text{for } \; j = n-1, n-2, \cdots, 1, 0, \end{aligned}$$

Moreover, the evaluation of $Q(x_k)$ can be obtained through the nested expression:

$$Q(x) = b_1 + x\left(b_2 + x\left(b_3 + \cdots + x\left(b_{n-1} + x b_n\right)\right)\right)$$

that is, let $c_n = b_n (= a_n)$, and for $j = n-1, n-2, \cdots, 1$,

$$c_j = b_j + c_{j+1}x_k,$$

then $Q(x_k) = c_1$.

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Horner's method (Evaluate $P(x_k)$ and $P'(x_k) = Q(x_k)$)

Set $y = a_n$; $z = a_n$ $(b_n = a_n;\ c_n = a_n)$.
For $j = n-1, n-2, \cdots, 1$
  Set $y = a_j + yx_k$; $z = y + zx_k$ $(b_j = a_j + b_{j+1}x_k;\ c_j = b_j + c_{j+1}x_k)$.
End for
Set $y = a_0 + yx_k$ $(b_0 = a_0 + b_1 x_k)$.
Output $P(x_k) = y$ $(= b_0)$; $P'(x_k) = z$ $(= c_1)$.

If x_N is an approximate zero of P, then

$$
\begin{aligned}
P(x) &= (x - x_N)Q(x) + b_0 = (x - x_N)Q(x) + P(x_N) \\
&\approx (x - x_N)Q(x) \equiv (x - \hat{x}_1)Q_1(x).
\end{aligned}
$$

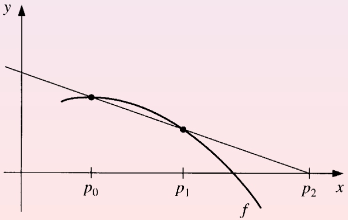
So $x - \hat{x}_1$ is an approximate factor of $P(x)$ and we can find a second approximate zero of P by applying Newton's method to $Q_1(x)$. The procedure is called deflation.

• Müller's method: Find complex roots of a polynomial $P(x)$ (or any complex valued function $f : \mathbb{C} \mapsto \mathbb{C}$):

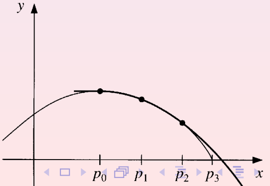
Theorem

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

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

It follows that

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

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

$$p_3 - p_2 = \frac{2c}{b \pm \sqrt{b^2 - 4ac}}. \tag{8}$$

If a, b, c are all real, we can choose

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

such that the denominator will be largest in magnitude. The selected p_3 is the one closer to p_2 among those given in (8).
In case a, b, c are complex, the selection principle for p_3 can be modified accordingly.

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 $i \leq M$

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

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