Computer-Assisted Problem-Solving / Numerical Methods

Root-Finding Methods

version: February 12th, 2020

Legend: Method, Theory, Example, Advanced, Appendix

Method

Bisection Method

Algorithm to solve $f(x) = 0$

1. **Calculate $m = \frac{a+b}{2}$ and $f(m)$**
2. **If $f(m) = 0$ we have found a zero. Done.**
3. **If $f(a) * f(m) < 0$ move right border: $b = m$**
   If $f(a) * f(m) > 0$ move left border: $a = m$
4. **If $|a - b| < \epsilon$ accuracy is sufficient. Take $m = \frac{a+b}{2}$ ($\Longrightarrow$ maximum error $\epsilon/2$). Done.**
5. **Go to step (1).**

Increase of accuracy after n iterations:

$$\text{Interval length} = \left(\frac{1}{2}\right)^n (b - a)$$

For $n = 10$: $(\frac{1}{2})^{10} \approx 10^{-3}$

$$\Longrightarrow \text{3 extra significant digits}$$

"linear convergence with factor 1/2"

Theory

Convergence Order and Factor

Let $x = p$ **is true solution of** $f(x) = 0$
Convergence: iterations $x_n \to p$
Error at iteration n **:** $\epsilon_n = |x_n - p|$
Error behaviour: $\epsilon_{n+1} = K{\epsilon_n}^{\alpha}$
Method converges with Order α **and Factor** K

Example

Example Bisection Method

Calculate $\sqrt{2} = 1.4142135623...$ **via** $f(x) = x^2 - 2 = 0$

Start interval $[1, 2]$

n	a_n	b_n	$x_n = m$
0	**1**	**2**	**1.5**
1	**1**	**1.5**	**1.25**
2	**1.25**	**1.5**	**1.375**
3	**1.375**	**1.5**	**1.4375**
4	**1.375**	**1.4375**	**1.40625**
5	**1.40625**	**1.4375**	**1.421875**
6	**1.40625**	**1.421875**	**1.414063**
7	**1.414063**	**1.421875**	**1.417969**
8	**1.414063**	**1.417969**	**1.416016**
9	**1.414063**	**1.416016**	**1.415040**
10	**1.414063**	**1.415040**	**1.414552**

3 extra significant digits at $n = 10$

Method

Successive Substitution Method

Re-formulate problem: $f(x) = 0 \Longrightarrow x = g(x)$

Iterative method: $x_n = g(x_{n-1})$

Example

Example Successive Substitution

Calculate zero(s) of $f(x) = x^2 - 3x + 1$

Answer: $x = \frac{3}{2} \pm \frac{1}{2}\sqrt{5} \approx 2.618034$ **or** $x \approx 0.381966$

Options: $g_1(x) = \frac{1}{3}(x^2 + 1)$, $g_2(x) = 3 - 1/x$, **etc.**

Starting values: $x_0 = 1$ **or** $x_0 = 3$

	$g_1(x) = \frac{1}{3}(x^2 + 1)$		$g_2(x) = 3 - \frac{1}{x}$	
n	$x_0 = 1$	$x_0 = 3$	$x_0 = 1$	$x_0 = 3$
0	**1**	**3**	**1**	**3**
1	**0.666667**	**3.333333**	**2.000000**	**2.666667**
2	**0.481481**	**4.037037**	**2.500000**	**2.625000**
3	**0.410608**	**5.765889**	**2.600000**	**2.619048**
4	**0.389533**	**11.415160**	**2.615385**	**2.618182**
5	**0.383912**	**43.768626**	**2.617647**	**2.618056**
6	**0.382463**	**...**	**2.617978**	**2.618037**
7	**0.382093**	**...**	**2.618026**	**2.618034**
8	**0.381998**	**...**	**2.618033**	**2.618034**
9	**0.381974**	**...**	**2.618034**	**2.618034**

Theory

Convergence Theorem

Convergence Theorem Successive Substitution

If:

1) $x = p$ **is a solution of** $x = g(x)$

2) $g(x)$ **has continuous derivative in interval** I **around** p

3) $|g'(x)| \leq K < 1$ **in I**

Then:

Successive substitution converges for arbitrary starting values in I **with convergence rate** K

Proof:

Mean Value Theorem (See Appendix) $\Longrightarrow$

$\exists\, t \in [x\,,\, p]$ **such that:**

$$g(x) - g(p) = g'(t)(x - p).$$

Furthermore $g(p) = p$ **and** $x_n = g(x_{n-1})$

Using $|g'(x)| \leq K < 1$ **it follows that**

$$|x_n - p| = |g(x_{n-1}) - g(p)| = |g'(t)||x_{n-1} - p| \leq K|x_{n-1} - p|$$

So that $$\epsilon_n \leq K\epsilon_{n-1}$$

with $\epsilon_n = |x_n - p|$ **the error at iteration step** n

Theory

Order of Convergence

Taylor-expansion around $x = p$:

$$x_{n+1} = g(x_n) = g(p)+g'(p)(x_n-p)+\frac{1}{2}g''(p)(x_n-p)^2+\ldots$$

Error in iteration n: $\epsilon_n = x_n - p$

By definition: $g(p) = p$

Therefore:

$$\epsilon_{n+1} = g'(p)\epsilon_n + \frac{1}{2}g''(p)\epsilon_n^2 + \ldots$$

If $g'(p) \neq 0$:

$\Longrightarrow$ **linear convergence:** $\epsilon_{n+1} \sim \beta_1\,\epsilon_n$, **with** $\beta_1 = g'(p)$

If $g'(p) = 0$ and $g''(p) \neq 0$:

$\Longrightarrow$ **quadratic conv. :** $\epsilon_{n+1} \sim \beta_2\,\epsilon_n^2$, **with** $\beta_2 = \frac{1}{2}g''(p)$

Example

Example Successive Substitution

Find the zero of $f(x) = x^3 + 2x^2 + 10x - 20$

Redefine problem: $x = g(x)$ **with**

$$g(x) = \frac{20}{x^2 + 2x + 10}$$

$$g'(x) = -40\frac{x+1}{(x^2 + 2x + 10)^2}$$

It follows that:

$$\left.\begin{array}{l} g'(x) = 0 \ \text{ if } \ x = -1 \\ g'(x) > 0 \ \text{ if } \ x < -1 \\ g'(x) < 0 \ \text{ if } \ x > -1 \end{array}\right\} \Longrightarrow g'(x) = 0 \text{ only in } x = -1$$

$x = -1$ **is not a fixed point of** $g(x) \Longrightarrow$

linear convergence? (no quadratic convergence)

Initial value $x_0 = 1 \Longrightarrow$

$|g'(x_0)| = |g'(1)| \approx |-0.47| < 1 \Longrightarrow$ **convergence!**

(if one starts close enough to the zero point)

n	x_n	$x_n - x_{n-1}$	$\frac{x_n - x_{n-1}}{x_{n-1} - x_{n-2}}$
0	**1**		
1	**1.53846**	$+$ **0.53846**	
2	**1.29502**	**- 0.24344**	**- 0.45**
3	**1.40183**	$+$ **0.10681**	**- 0.44**
4	**1.35421**	**- 0.04762**	**- 0.45**
5	**1.37530**	$+$ **0.02109**	**- 0.44**
6	**1.36593**	**- 0.00937**	**- 0.44**
7	**1.37009**	$+$ **0.00416**	**- 0.44**
8	**1.36824**	**- 0.00185**	**- 0.44**
9	**1.36906**	$+$ **0.00082**	**- 0.44**
10	**1.36870**	**- 0.00036**	**- 0.44**
11	**1.36886**	$+$ **0.00016**	**- 0.44**

Solution: $p \approx 1.3688$**.**

Leonardo of Pisa (Fibonacci; 1225 A.D.):

$p = 1.368808107$

Convergence rate: $\tilde{K} \approx -0.44$

This equals: $g'(p) \approx g'(1.4) \approx -0.44$**, since**

$$\epsilon_{n+1} = g'(p)\epsilon_n + \ldots$$

Theory

Error Estimates

Convergence rate $\tilde{K} = \frac{x_n - x_{n-1}}{x_{n-1} - x_{n-2}}$:

$$\epsilon_n = \tilde{K}\epsilon_{n-1} = (1+\tilde{K})\epsilon_{n-1} - \tilde{K}\frac{\epsilon_{n-1}}{\tilde{K}} \Longrightarrow$$

$$\epsilon_n = (1+\tilde{K})\epsilon_{n-1} - \tilde{K}\epsilon_{n-2} \Longrightarrow$$

$$\epsilon_n - \epsilon_{n-1} = \tilde{K}(\epsilon_{n-1} - \epsilon_{n-2}) \Longrightarrow$$

$$(x_n - p) - (x_{n-1} - p) = \tilde{K}[(x_{n-1} - p) - (x_{n-2} - p)] \Longrightarrow$$

$$\tilde{K} = \frac{x_n - x_{n-1}}{x_{n-1} - x_{n-2}}$$

Error estimate 1:

$$|(x_n - p)| = |(x_{n+1} - p) + (x_n - x_{n+1})| \leq$$

$$|(x_{n+1} - p)| + |(x_n - x_{n+1})| \leq K|(x_n - p)| + |(x_n - x_{n+1})| \Longrightarrow$$

$$|(x_n - p)| \leq \frac{1}{1-K}|(x_n - x_{n+1})|$$

Use this to estimate the error:

$$\epsilon_n \leq \frac{1}{1-K}|(x_n - x_{n+1})|$$

$$\Longrightarrow \epsilon_{n+1} \leq K\epsilon_n \leq \frac{K}{1-K}|(x_n - x_{n+1})|$$

Error estimate 2 (use K repeatedly):

$$|(x_{n+1} - x_n)| = |g(x_n) - g(x_{n-1})| \leq K|x_n - x_{n-1}| = \ldots$$

$$\leq K^n|x_1 - x_0| \Longrightarrow \epsilon_n \leq \frac{K^n}{1-K}|(x_1 - x_0)|$$

Method

Newton's Method

Taylor expansion around $x = x_n$:

$$f(x_{n+1}) = f(x_n) + (x_{n+1} - x_n) f'(x_n) + \frac{(x_{n+1} - x_n)^2}{2} f''(x_n) + \ldots$$

Goal:

new value x_{n+1} is a good approximation of the zero: $f(x_{n+1}) \approx 0$

If $x_{n+1} - x_n$ small $\Longrightarrow$ neglect 2nd and higher order

$$f(x_{n+1}) = f(x_n) + (x_{n+1} - x_n) f'(x_n) \approx 0$$

Newton's Method:

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

Conditions: $f'(x)$ **exists and is continuous**
$f'(x) \neq 0$ **for** $x \approx x_n$

Example

Example Newton's Method

Find $\sqrt{2}$ **via** $f(x) = x^2 - 2 = 0$

Initial value $x_0 = 1$

$f'(x) = 2x \Longrightarrow$

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

n	x_n
0	**1**
1	**1.500000**
2	**1.416667**
3	**1.414216**
4	**1.414214**

Correct value: $\sqrt{2} = 1.41421356237...$

After 4 iterations already 6 correct digits!

Heron's rule (Heron of Alexandria; 10–70 A.D.)

Theory

Convergence Newton's Method

Method satisfies $x_{n+1} = g(x_n)$**, with**

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

First derivative:

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

At the zero $x = p$**:** $f(p) = 0 \Longrightarrow g'(p) = 0$

Second derivative: $g''(p) = f''(p)/f'(p) \neq 0$
(check yourself)

Consequence:
if convergence, then quadratic convergence

For convergence still $|g'(x)| \leq 1$ **required near zero** $x = p$

Theory

Problems with Newton

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

Possible Problems:

1: $f'(x)$ **computationally expensive**

2: $f'(x) \approx 0 \Longrightarrow$ **number loss**

may hamper convergence

3: $f'(x) = 0$

Multiple roots:

$f(x) = (x-p)^n \, h(x) \quad (n > 1) \;\Longrightarrow$

$f'(x) = n\,(x-p)^{(n-1)}\, h(x) \;+\; (x-p)^n\, h'(x) \;\Longrightarrow$

$f'(p) = 0$

First derivative of $g(x)$ function:

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

$$g'(p) = \cdots = \frac{(n-1)}{n}$$

For $n > 1$ no 2nd order convergence: $g'(p) \neq 0$

Example

Example Fixed Point methods

Solve: $\sin(x) + x^2 = 2$ **for** $x > 0$

A plot shows $x \approx 1$

Find zero: $f(x) = \sin(x) + x^2 - 2 = 0$

1) Successive Substitution:

$$g(x) = \alpha(\sin(x) + x^2 - 2) + x$$

Conditions for α**:**

$$g'(x) = \alpha\,(\cos(x) + 2x) + 1 \Longrightarrow |g'(1)| \approx |2.5\,\alpha + 1|$$

$$|g'(1)| < 1 \Longleftrightarrow -0.8 < \alpha < 0$$

$$|g'(1)| \text{ minimum if } \alpha = -0.4 \;(\Rightarrow \text{fast method})$$

Iteration rule:

$$x_{n+1} = g(x_n) = \alpha\,(\sin(x_n) + x_n^2 - 2) + x_n$$

2) Newton's Method:

Iteration rule:

$f'(x) = \cos(x) + 2x \Longrightarrow$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{\sin(x_n) + x_n^2 - 2}{\cos(x_n) + 2x_n}$$

Solution of $\sin(x) + x^2 = 2$ **for** $x > 0$

n	$\alpha = -7/10$	$\alpha = -4/10$	**Newton**
0	**1.0**	**1.0**	**1.0**
1	**1.11097031**	**1.06341161**	**1.06240557**
2	**1.01970098**	**1.06146661**	**1.06154993**
3	**1.09548188**	**1.06155345**	**1.06154977**
4	**1.03302129**	**1.06154961**	**1.06154977**
5	**1.08483286**	**1.06154978**	**1.06154977**
6	**1.04207148**	**1.06154977**	**1.06154977**
7	**1.07751670**	**1.06154977**	**1.06154977**
8	**1.04823788**	**1.06154977**	**1.06154977**
9	**1.07249445**	**1.06154977**	**1.06154977**
10	**1.05244661**	**1.06154977**	**1.06154977**
11	**1.06904931**	**1.06154977**	**1.06154977**
12	**1.05532225**	**1.06154977**	**1.06154977**
13	**1.06668732**	**1.06154977**	**1.06154977**
14	**1.05728839**	**1.06154977**	**1.06154977**

Newton: vary fast (quadratic convergence)

Successive Substitution:

1) fast convergence for $\alpha = -0.4$ $(K \approx 0)$

2) 100 iterations needed if $\alpha = -0.7 (K \approx 0.75 < 1)$

Method

Secant Method

Alternative for Newton

Approximation of derivative

$$f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

$$\textbf{Newton}: \quad x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \Longrightarrow$$

$$\textbf{Secant}: \quad x_{n+1} = x_n - f(x_n)\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}$$

Be efficient: store x_{n-1} and $f(x_{n-1})$

Only one function call needed: $f(x_n)$

Advantage: $f'(x_n)$ not needed

Disadvantage: not 2nd order anymore

Convergence order:

$\alpha = \frac{1}{2}(1 + \sqrt{5}) \approx 1.618$ **(golden ratio)**

(so better than 1st order !)

Example

Example: Secant vs. Newton

Example: $f(x) = x^6 - x - 1$ **and** $x_0 = 2$

Solution: 1.134724138401519

Secant

n	x_n	ϵ_n	$x_n - x_{n-1}$
1	1.00000000	1.347E−01	−1.000E+00
2	1.01612903	1.186E−01	1.613E−02
3	1.19057777	−5.585E−02	1.744E−01
4	1.11765583	1.707E−02	−7.292E−02
5	1.13253155	2.193E−03	1.488E−02
6	1.13481681	−9.267E−05	2.285E−03
7	1.13472365	4.925E−07	−9.316E−05
8	1.13472414	1.103E−10	4.923E−07
9	1.13472414	−1.319E−16	1.103E−10

Newton

n	x_n	ϵ_n	$x_n - x_{n-1}$	$(\epsilon_n)/(\epsilon_{n-1})^2$
1	1.68062827	−5.459E−01	−3.194E−01	−7.291E−01
2	1.43073899	−2.960E−01	−2.499E−01	−9.933E−01
3	1.25497096	−1.202E−01	−1.758E−01	−1.372E+00
4	1.16153843	−2.681E−02	−9.343E−02	−1.854E+00
5	1.13635327	−1.629E−03	−2.519E−02	−2.266E+00
6	1.13473053	−6.390E−06	−1.623E−03	−2.408E+00
7	1.13472414	−9.870E−11	−6.390E−06	−2.417E+00
8	1.13472414	2.220E−16	−9.870E−11	2.279E+04
9	1.13472414	2.220E−16	0.000E+00	4.504E+15

Advanced

Aitken/Steffensen Acceleration

Make use of linear convergence:

$$\frac{\epsilon_n}{\epsilon_{n-1}} \approx \frac{\epsilon_{n-1}}{\epsilon_{n-2}} \Longrightarrow \frac{p - x_n}{p - x_{n-1}} \approx \frac{p - x_{n-1}}{p - x_{n-2}}$$

$\Longrightarrow$**Approximation for solution**

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

Aitken extrapolation (improved solution)

$$\hat{x}_{n-2} = x_{n-2} - \frac{(x_{n-1} - x_{n-2})^2}{x_n - 2x_{n-1} + x_{n-2}}$$

Aitken error estimation (backward)

$$\epsilon_{n-2} = |p - x_{n-2}| \approx \frac{(x_{n-1} - x_{n-2})^2}{x_n - 2x_{n-1} + x_{n-2}}$$

Alternative by Steffensen (forward)

$$\frac{\epsilon_{n-1}}{\epsilon_n} \approx \frac{\epsilon_{n-2}}{\epsilon_{n-1}} \Longrightarrow \frac{p - x_{n-1}}{p - x_n} \approx \frac{p - x_{n-2}}{p - x_{n-1}} \Longrightarrow$$

Extrapolation $\quad p \approx \hat{x}_n = x_n - \dfrac{(x_{n-1} - x_n)^2}{x_{n-2} - 2x_{n-1} + x_n}$

Error Estimation $\epsilon_n = |p - x_n| \approx \dfrac{(x_{n-1} - x_n)^2}{x_{n-2} - 2x_{n-1} + x_n}$

Comparable to estimate: $\epsilon_{n+1} \leq \frac{K}{1-K}|(x_n - x_{n+1})|$

Example

Example Steffensen

$6.28+\sin(x)-x = 0$, **solution:** $p = 6.0155030729454921\ldots$

Method: $x_{n+1} = 6.28 + \sin(x_n)$, **with** $x_0 = 6$

Steffensen Error Estimation

n	x_n	$x_n - x_{n-1}$	$\tilde{K}_n$	$p - x_n$	err.est.
0	6.00000000			1.550L–02	
1	6.00058450	5.845L–04		1.492L–02	
2	6.00114577	5.613L–04	0.9603	1.436L–02	1.356L–02
3	6.00168482	5.390L–04	0.9604	1.382L–02	1.308L–02
4	6.00220261	5.178L–04	0.9606	1.330L–02	1.261L–02
5	6.00270006	4.974L–04	0.9607	1.280L–02	1.216L–02
6	6.00317803	4.780L–04	0.9609	1.233L–02	1.173L–02
7	6.00363736	4.593L–04	0.9610	1.187L–02	1.131L–02
8	6.00407883	4.415L–04	0.9611	1.142L–02	1.091L–02
9	6.00450319	4.244L–04	0.9612	1.100L–02	1.052L–02

Steffensen Extrapolation

n	x_n	$x_n - x_{n-1}$	$\tilde{K}_n$	$p - x_n$	
0	6.00000000			1.550L–02	
1	6.00058450	5.845L–04		1.492L–02	
2	6.00114577	5.613L–04	0.9603	1.436L–02	
∗ 3	6.01470515	1.356L–02		7.979L–04	∗accel
4	6.01473365	2.850L–05		7.694L–04	
5	6.01476113	2.748L–05	0.9642	7.419L–04	
∗ 6	6.01550080	7.397L–04		2.271L–06	∗accel
7	6.01550088	8.088L–08		2.190L–06	
8	6.01550096	7.800L–08	0.9644	2.112L–06	
∗ 9	6.01550307	2.112L–06		–5.409L–12	∗accel

Acceptable error estimation

Weak linear convergence $\tilde{K}_n \approx 0.96$

Extrapolation at $*$ **really helps!**

Extrapolation $\Rightarrow$ **almost 2nd order convergence**

Appendix

Mean Value Theorem

Rolle's Theorem:

Suppose $h(x)$ **on** $[a, b]$ **is continuous,**

with end points $h(a) = h(b)$

There must be a c **in** $[a, b]$ **such that:** $h'(c) = 0$

Define $h(x) = f(x) - f(a) - \dfrac{f(b) - f(a)}{b - a}(x - a)$

Then: $h(a) = h(b) = 0$

Rolle $\Longrightarrow$ $h'(c) = 0$ **somewhere in** $[a, b]$

Differentiation

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

At location $x = c$

$$h'(c) = f'(c) - \frac{f(b) - f(a)}{b - a}$$

Then $h'(c) = 0 \Longrightarrow$

$$f'(c) = \frac{f(b) - f(a)}{b - a}$$

And finally $f(b) - f(a) = f'(c)(b - a)$