4. Roots of equations: open methods

- fixed point iteration
- Newton-Raphson
- secant method
- modified Newton-Raphson

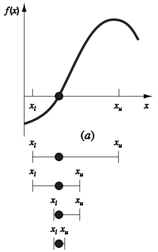
Open versus bracketing methods

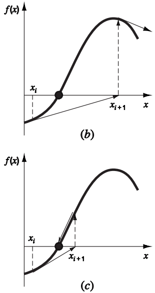
Bracketing methods

- start with $[x_l, x_u]$ where $f(x_l)f(x_u) < 0$
- repeated halving/refinement $\Rightarrow$ always convergent (moves closer to the true root)

Open methods

- use formulas with one start value or two that need not bracket the root
- may *diverge* (move away from the true root)
- when they converge, they typically do so *faster* than bracketing methods





Fixed-point iteration

rearrange $f(x) = 0$ into *fixed-point* form

$$x = g(x)$$

- for example
  - algebraic manipulation: $x^2 - 2x + 3 = 0 \;\Rightarrow\; x = \dfrac{x^2 + 3}{2}$
  - add x to both sides: $\sin x = 0 \;\Rightarrow\; x = x + \sin x$
- given an initial guess x_0, iterate

$$x_{i+1} = g(x_i), \quad i = 0, 1, \ldots$$

  called *fixed point iteration* (or *one-point iteration* or *successive substitution*)

- monitor the approximate relative error

$$\varepsilon_a = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| \times 100\%$$

Example

$$f(x) = e^{-x} - x$$

true root: $x^\star \approx 0.56714329$

separate directly and iterate $x_{i+1} = e^{-x_i}$ with $x_0 = 0$

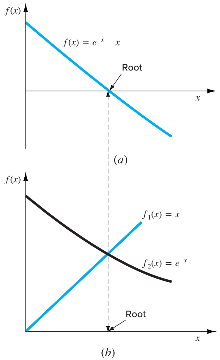
i	x_i	ε_a (%)	ε_t (%)
0	0.000000		100.0
1	1.000000	100.0	76.3
2	0.367879	171.8	35.1
3	0.692201	46.9	22.1
4	0.500473	38.3	11.8
5	0.606244	17.4	6.89
6	0.545396	11.2	3.83
7	0.579612	5.90	2.20
8	0.560115	3.48	1.24
9	0.571143	1.93	0.705
10	0.564879	1.11	0.399

Two-curve graphical method

- split $f(x) = f_1(x) - f_2(x) = 0$ into $y_1 = f_1(x)$ and $y_2 = f_2(x)$
- the intersections give roots

Example: for $e^{-x} - x = 0$, take $y_1 = x$, $y_2 = e^{-x}$

x	$y_1 = x$	$y_2 = e^{-x}$
0.0	0.000	1.000
0.2	0.200	0.819
0.4	0.400	0.670
0.6	0.600	0.549
0.8	0.800	0.449
1.0	1.000	0.368



intersection near $x \approx 0.57$

Convergence via two-curve method

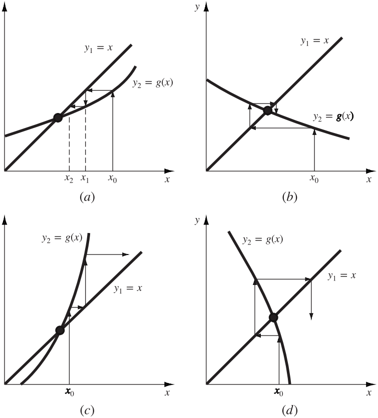
the two-curve method can be used to illustrate convergence and divergence

- equation $x = g(x)$ is re-expressed as a pair of equations: $y_1 = x,\ y_2 = g(x)$
- roots of $f(x) = 0$ correspond to the abscissa at the intersection of the two curves
- function $y_1 = x$ and $y_2 = g(x)$ are plotted

Iteration procedure

- start with initial guess x_0
- determine the corresponding point on y_2 curve: $(x_0, g(x_0))$
- move horizontally to y_1: the point (x_1, x_1)
- this corresponds to the first fixed-point iteration: $x_1 = g(x_0)$
- repeat starting from x_1

Convergence via two-curve method



- (a) and (b): solution converges — estimates move closer to the root
- (c) and (d): iterations diverge away from the root

Convergence

fixed-point iteration converges locally (in a region of interest) if

$$|g'(x)| < 1$$

meaning the slope of $y_2 = g(x)$ is less than the slope of $y_1 = x$

- $0 < g'(x^\star) < 1$: monotone convergence
- $-1 < g'(x^\star) < 0$: oscillatory (spiral) convergence
- $|g'(x^\star)| > 1$: divergence

Proof: mean-value theorem with $x_{i+1} = g(x_i)$, $x^\star = g(x^\star)$:

$$x^\star - x_{i+1} \;=\; g(x^\star) - g(x_i) \;=\; g'(\xi)\,(x^\star - x_i)$$

thus for the true error $E_{t,i} = x^\star - x_i$,

$$E_{t,i+1} = g'(\xi)\,E_{t,i} \quad \Rightarrow \quad |g'(\xi)| < 1 \;\Rightarrow\; |E_{t,i+1}| < |E_{t,i}|$$

if converges, error decreases proportional to each step (linear convergence)

MATLAB code of our example

```
clear,clc,format compact
g=@(x) exp(-x);
x0 = 0;
[xr,ea,iter] = fixpt(g,x0,1e-6);
X = ['The root = ',num2str(xr),' (ea = ',num2str(ea),'% in ',...
num2str(iter),' iterations)'];
disp(X)
```

with function

```
function [x1,ea,iter] = fixpt(g,x0,es,maxit)
% fixpt: fixed point root locator
if nargin < 2, error('at least 2 arguments required'), end
if nargin < 3||isempty(es),es = 1e-6;end % if es is blank set to 1e-6
if nargin < 4||isempty(maxit),maxit = 50;end % if maxit is blank set to 50
iter = 0; ea = 100;
while (1)
x1 = g(x0);
iter = iter + 1;
if x1 ~= 0, ea = abs((x1 - x0)/x1)*100; end
if (ea <= es || iter >= maxit), break, end
x0 = x1;
end
end
```

Outline

- fixed point iteration
- **Newton-Raphson**
- secant method
- modified Newton-Raphson

Newton-Raphson method

- first-order Taylor approximation around x_i

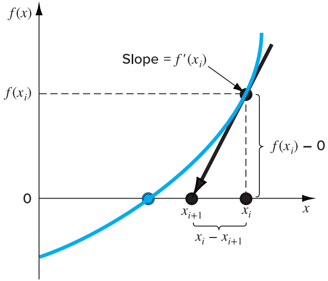
$$f(x) \approx \hat{f}(x) = f(x_i) + f'(x_i)(x - x_i)$$

- set to zero $\hat{f}(x) = 0$:

$$0 = f(x_i) + f'(x_i)(x - x_i)$$

- solution is our next estimate:

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$



called *Newton-Raphson method* or just *Newton method*

Example

use the Newton-Raphson method to estimate the root of

$$f(x) = e^{-x} - x$$

starting with an initial guess of $x_0 = 0$ (true root: $x^\star \approx 0.56714329$)

- first derivative:

$$f'(x) = -e^{-x} - 1$$

- iterative equation:

$$x_{i+1} = x_i - \frac{e^{-x_i} - x_i}{-e^{-x_i} - 1}$$

Example

first iteration:

$$x_1 = x_0 - \frac{e^{-x_0} - x_0}{-e^{-x_0} - 1} = 0 - \frac{e^{-0} - 0}{-e^{-0} - 1} = 0.5$$

repeating gives the results

i	x_i	$\varepsilon_t(\%)$	E_t
0	0.000000000	100.0	0.567143290
1	0.500000000	11.8	0.067143290
2	0.566311003	0.147	0.000832287
3	0.567143165	0.0000221	0.000000125
4	0.567143290	$< 10^{-8}$	0.000000000

converges much faster than fixed-point iteration

Error analysis of Newton-Raphson

second-order Taylor approximation:

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

setting $x = x^\star$ and using $f(x^\star) = 0$ gives

$$0 = f(x_i) + f'(x_i)(x^\star - x_i) + \frac{f''(\xi)}{2!}(x^\star - x_i)^2$$

subtracting from Newton update $0 = f(x_i) + f'(x_i)(x_{i+1} - x_i)$ gives

$$0 = f'(x_i)(x^\star - x_{i+1}) + \frac{f''(\xi)}{2!}(x^\star - x_i)^2$$

define error $E_{t,i+1} = x^\star - x_{i+1}$ and assume convergence ($x_i, \xi \to x^\star$):, we get

$$E_{t,i+1} \approx -\frac{f''(x^\star)}{2f'(x^\star)}\, E_{t,i}^2$$

- error decreases quadratically
- number of correct digits roughly doubles with each iteration

Example

examine error of Newton-Raphson for $f(x) = e^{-x} - x$, at $x^\star = 0.56714329$

we have

$$f'(x^\star) = -1.56714329, \quad f''(x^\star) = 0.56714329$$

- error factor: $E_{t,i+1} \approx -\frac{f''(x^\star)}{2f'(x^\star)} E_{t,i}^2 = 0.18095 E_{t,i}^2$
- initial error with $x_0 = 0$: $E_{t,0} = 0.56714329$
- predicted errors using $E_{t,i+1} \approx 0.18095\, E_{t,i}^2$:

$$\begin{aligned}
E_{t,1} &\approx 0.0582 \quad \text{(true: } 0.0671) \\
E_{t,2} &\approx 8.16 \times 10^{-4} \quad \text{(true: } 8.32 \times 10^{-4}) \\
E_{t,3} &\approx 1.25 \times 10^{-7} \\
E_{t,4} &\approx 2.84 \times 10^{-15}
\end{aligned}$$

- confirms quadratic convergence: error shrinks $\propto E_{t,i}^2$

Example

determine the positive root of $f(x) = x^{10} - 1$ using Newton-Raphson with $x_0 = 0.5$

Newton-Raphson update

$$x_{i+1} = x_i - \frac{x_i^{10} - 1}{10x_i^9}$$

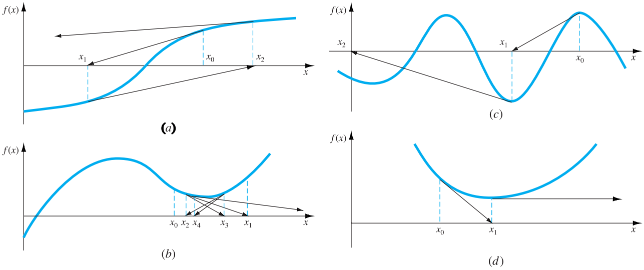
Iterations

i	x_i
0	0.5
1	51.65
2	46.485
3	41.8365
4	37.65285
5	33.887565
$\vdots$	$\vdots$
∞	1.0000000

very slow convergence

Pitfalls of Newton-Raphson

- can be slow and may diverge
- *inflection points:* if $f''(x) = 0$ near a root, iterations may diverge (figure a)
- *oscillations:* iterations can bounce around local maxima/minima (figure b)
- *near-zero slopes:* lead to very large jumps, possibly to other roots (figure c)
- *division by zero:* if $f'(x) = 0$, iteration fails completely (figure d)



Convergence insights

- no universal convergence guarantee
- success depends on:
  - nature of the function
  - quality of the initial guess
- remedies:
  - choose initial guesses close to the root
  - use graphical insight or physical intuition
  - use small stepsize $\alpha > 0$:

$$x_{i+1} = x_i - \alpha \frac{f(x_i)}{f'(x_i)}$$

  - design software to detect slow convergence or divergence

Outline

- fixed point iteration
- Newton-Raphson
- **secant method**
- modified Newton-Raphson

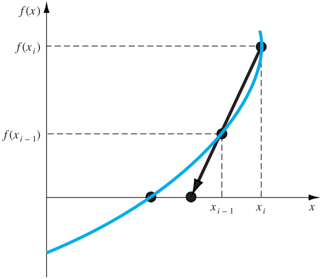
Secant method

- some functions have derivatives that are difficult or inconvenient to evaluate
- the derivative can be approximated by a backward finite divided difference

$$f'(x_i) \approx \frac{f(x_{i-1}) - f(x_i)}{x_{i-1} - x_i}$$

this approximation can be substituted into to yield the **secant method:**

$$x_{i+1} = x_i - \frac{f(x_i)(x_{i-1} - x_i)}{f(x_{i-1}) - f(x_i)}$$



Example

use the secant method on $f(x) = e^{-x} - x$ with starting points $x_{-1} = 0$, $x_0 = 1.0$

true root ≈ 0.56714329

First iteration

$$x_{-1} = 0 \quad f(x_{-1}) = 1.00000$$

$$x_0 = 1 \quad f(x_0) = -0.63212$$

so

$$x_1 = 1 - \frac{-0.63212(0-1)}{1-(-0.63212)} = 0.61270 \quad \varepsilon_t = 8.0\%$$

Example

Second iteration

$$x_0 = 1 \quad f(x_0) = -0.63212$$

$$x_1 = 0.61270 \quad f(x_1) = -0.07081$$

note both estimates are now on the same side of the root; we have

$$x_2 = 0.61270 - \frac{-0.07081(1 - 0.61270)}{-0.63212 - (-0.07081)} = 0.56384 \quad \varepsilon_t = 0.58\%$$

Third iteration

$$x_1 = 0.61270 \quad f(x_1) = -0.07081$$

$$x_2 = 0.56384 \quad f(x_2) = 0.00518$$

so

$$x_3 = 0.56384 - \frac{0.00518(0.61270 - 0.56384)}{-0.07081 - (-0.00518)} = 0.56717 \quad \varepsilon_t = 0.0048\%$$

Secant method versus false-position method

false position

$$x_r = x_u - \frac{f(x_u)\,(x_l - x_u)}{f(x_l) - f(x_u)}$$

secant

$$x_{i+1} = x_i - \frac{f(x_i)(x_{i-1} - x_i)}{f(x_{i-1}) - f(x_i)}$$

- identical first iterate if $x_u = x_0$ and $x_l = x_{-1}$
- difference
  - false-position: always brackets the root by replacing the value with same sign as $f(x_r)$
  - secant: updates sequentially (x_{i+1} replaces x_i and x_i replaces x_{i-1})
- consequence
  - false-position: guaranteed convergence (root stays in bracket)
  - secant: may converge faster but can also diverge

Example

use false-position and secant methods to estimate the root of $f(x) = \ln x$

initial guesses: $x_l = x_{-1} = 0.5, x_u = x_0 = 5.0$

False-position iterations

iteration	x_l	x_u	x_r
1	0.5	5.0	1.8546
2	0.5	1.8546	1.2163
3	0.5	1.2163	1.0585

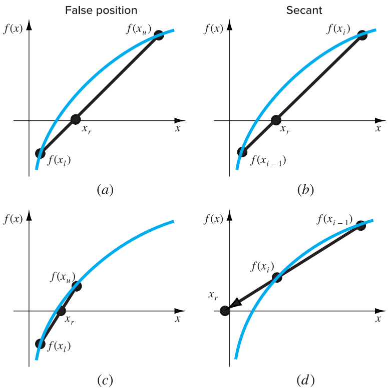
converges to true root $x = 1$

Secant iterations

iteration	x_{i-1}	x_i	x_{i+1}
1	0.5	5.0	1.8546
2	5.0	1.8546	-0.10438

result: divergence

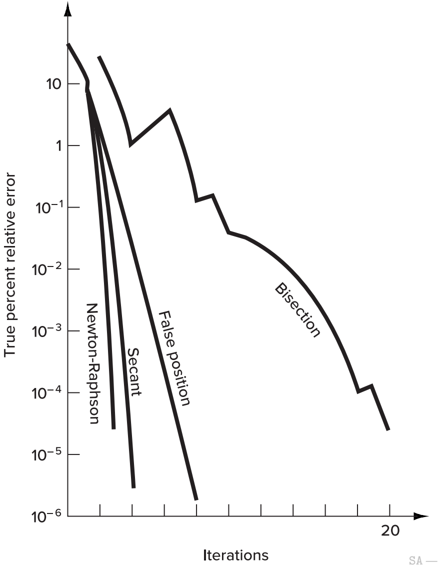
Example



- for secant both values lie on same side of the root
- false-position is robust but slower because one endpoint stays fixed
- secant usually converges faster when it works

Example: numerical comparison

comparison for $f(x) = e^{-x} - x$



Modified secant method

to avoid evaluating derivatives and two guesses

approximate derivative with perturbation δ:

$$f'(x_i) \approx \frac{f(x_i + \delta x_i) - f(x_i)}{\delta x_i}$$

iterative formula

$$x_{i+1} = x_i - \frac{\delta x_i f(x_i)}{f(x_i + \delta x_i) - f(x_i)}$$

- δ must be chosen carefully
  - too small $\longrightarrow$ subtractive cancellation
  - too large $\longrightarrow$ inefficiency or divergence
- useful when derivatives are difficult or inconvenient

Example: modified secant

use modified secant method to solve $f(x) = e^{-x} - x$, $\delta = 0.01$, $x_0 = 1.0$

- *first iteration*:

$$x_0 = 1, \quad f(x_0) = -0.63212$$
$$x_0 + \delta x_0 = 1.01, \quad f(x_0 + \delta x_0) = -0.64578$$
$$x_1 = 1 - \frac{0.01(-0.63212)}{-0.64578-(-0.63212)} = 0.537263, \quad |\varepsilon_t| = 5.3\%$$

- *second iteration*:

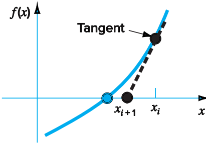
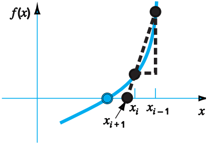
$$x_1 = 0.537263, \quad f(x_1) = 0.047083$$
$$x_1 + \delta x_1 = 0.542635, \quad f(x_1 + \delta x_1) = 0.038579$$
$$x_2 = 0.537263 - \frac{0.005373(0.047083)}{0.038579-0.047083} = 0.56701, \quad |\varepsilon_t| = 0.0236\%$$

- *third iteration*:

$$x_2 = 0.56701, \quad f(x_2) = 0.000209$$
$$x_2 + \delta x_2 = 0.572680, \quad f(x_2 + \delta x_2) = -0.00867$$
$$x_3 = 0.56701 - \frac{0.00567(0.000209)}{-0.00867-0.000209} = 0.567143, \quad |\varepsilon_t| = 2.365 \times 10^{-5}\%$$

- method converges rapidly to true root 0.56714329

Summary

Method	Formulation	Graphical Interpretation	Errors and Stopping Criteria
Newton-Raphson	$x_{i+1} = x_i - \dfrac{f(x_i)}{f'(x_i)}$		Stopping criterion: $\left\lvert \dfrac{x_{i+1} - x_i}{x_{i+1}} \right\rvert 100\% \le \epsilon_s$ Error: $E_{i+1} = O(E_i^2)$
Secant	$x_{i+1} = x_i - \dfrac{f(x_i)(x_{i-1} - x_i)}{f(x_{i-1}) - f(x_i)}$		Stopping criterion: $\left\lvert \dfrac{x_{i+1} - x_i}{x_{i+1}} \right\rvert 100\% \le \epsilon_s$

Outline

- fixed point iteration
- Newton-Raphson
- secant method
- **modified Newton-Raphson**

Multiple roots

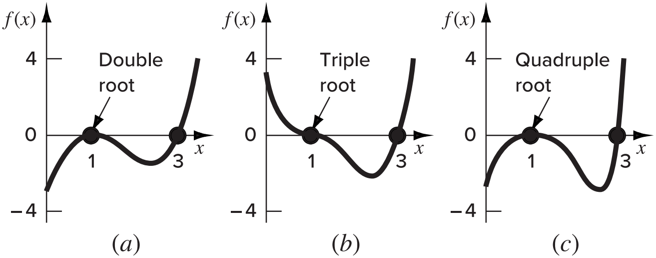
a **multiple root** occurs when a function is tangent to the x-axis at the root

- example: double root (touches the axis at $x = 1$ without crossing)

$$f(x) = (x-3)(x-1)(x-1) = x^3 - 5x^2 + 7x - 3$$

- example: triple root (tangent and crosses the axis at $x = 1$)

$$f(x) = (x-3)(x-1)^3 = x^4 - 6x^3 + 12x^2 - 10x + 3$$



- **rule of thumb**: even multiplicities touch but do not cross; odd multiplicities cross

Why multiple roots are tricky

1. **bracketing methods fail for even multiplicities:** f does not change sign, so bracketing tests may not detect the root
2. **derivative vanishes at the root:** $f'(x^\star) = 0$ as well as $f(x^\star) = 0$
   - Newton and secant divide by f' $\Rightarrow$ possible division by values near zero
   - practical safeguard: check $|f(x_i)|$ first and terminate when below tolerance (since f reaches 0 before f')
3. **slower convergence:** standard Newton and secant become *linearly* convergent for multiple roots

Modified Newton method

Modified Newton method for known multiplicity

$$x_{i+1} \;=\; x_i \;-\; m\,\frac{f(x_i)}{f'(x_i)}$$

- m is root multiplicity
- modify Newton to restore quadratic convergence
- requires prior knowledge of m

Modified Newton method: applies Newton to $u(x) = \frac{f(x)}{f'(x)}$

$$x_{i+1} = x_i - \frac{u(x_i)}{u'(x_i)} \;=\; x_i - \frac{f(x_i)f'(x_i)}{[f'(x_i)]^2 - f(x_i)f''(x_i)}$$

- $u(x) = \frac{f(x)}{f'(x)}$ has same roots as $f(x)$
- regains fast (quadratic) convergence at multiple roots

Example

use both the standard and modified Newton-Raphson to find the multiple root

$$f(x) = (x-3)(x-1)^2 = x^3 - 5x^2 + 7x - 3$$

- starting from $x_0 = 0$
- we have

$$f'(x) = 3x^2 - 10x + 7, \qquad f''(x) = 6x - 10$$

(standard) Newton

$$x_{i+1} = x_i - \frac{x_i^3 - 5x_i^2 + 7x_i - 3}{3x_i^2 - 10x_i + 7}$$

modified Newton

$$x_{i+1} = x_i - \frac{(x_i^3 - 5x_i^2 + 7x_i - 3)(3x_i^2 - 10x_i + 7)}{(3x_i^2 - 10x_i + 7)^2 - (x_i^3 - 5x_i^2 + 7x_i - 3)(6x_i - 10)}$$

Example: results

(standard) Newton

i	x_i	$\lvert\varepsilon_t\rvert$ (%)
0	0.0000000	100
1	0.4285714	57
2	0.6857143	31
3	0.8328654	17
4	0.9133290	8.7
5	0.9557833	4.4
6	0.9776551	2.2

behavior: steady but linear approach to $x^\star = 1$

modified Newton

i	x_i	$\lvert\varepsilon_t\rvert$ (%)
0	0.000000	100
1	1.105263	11
2	1.003082	0.31
3	1.000002	2.4×10^{-4}

behavior: rapid (quadratic) approach to $x^\star = 1$

Example

to estimate root $x = 3$, we start at $x_0 = 4$

standard Newton

i	x_i	$\lvert\varepsilon_t\rvert$ (%)
0	4.000000	33
1	3.400000	13
2	3.100000	3.3
3	3.008696	0.29
4	3.000075	2.5×10^{-3}
5	3.000000	2×10^{-7}

modified Newton

i	x_i	$\lvert\varepsilon_t\rvert$ (%)
0	4.000000	33
1	2.636364	12
2	2.820225	6.0
3	2.961728	1.3
4	2.998479	0.051
5	2.999998	7.7×10^{-5}

- for a simple root, standard Newton is slightly more efficient
- and requires fewer computation (no f'')

Modified secant method for multiple roots

- modified version of the secant method suited for multiple roots can also be developed
- apply secant method on $u(x) = f(x)/f'(x)$
- the resulting formula is:

$$x_{i+1} = x_i - \frac{u(x_i)\,(x_{i-1} - x_i)}{u(x_{i-1}) - u(x_i)}$$

References and further readings

- S. C. Chapra and R. P. Canale. *Numerical Methods for Engineers* (8th edition). McGraw Hill, 2021. (Ch.6)

- S. C. Chapra. *Applied Numerical Methods with MATLAB for Engineers and Scientists* (5th edition). McGraw Hill, 2023. (Ch.6)