Rootfinding

CHAPTER 2 of '***A first course in Computational Physics***', Paul L. DeVries, John Wiley & Sons (1994)

CHAPTER 3 of '***Elementary Numerical Analysis***', 3rd Edition, Kendall Atkinson and Weimin Han, John Wiley & Sons (2004)

Introduction

- Problem to be solved: $\boxed{f(x) = 0}$

for example: $a_0 + a_1 x + a_2 x^2 = 0$

- This type of problem occurs very frequently, for example maximization/minimization

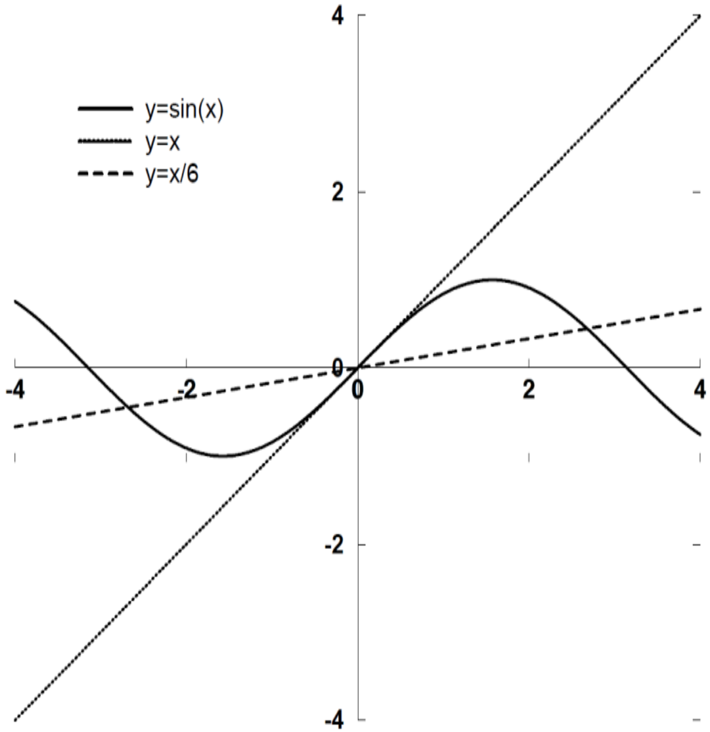
min energy: $\frac{\partial E(x)}{\partial x} = 0$ max entropy: $\frac{\partial S(x)}{\partial x} = 0$

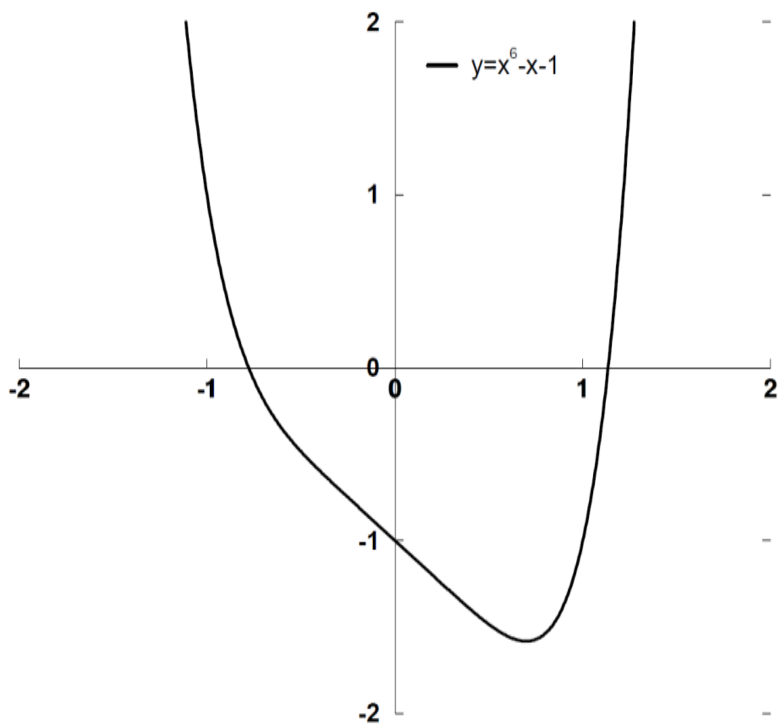
- Usually the problem cannot be solved analytically!

for example: $\sin(x) = ax$

Graphical approach

- First try to get as much insight as possible!





Bisection method

- Very robust and reliable
- Slow: see later for examples and error analysis

1. Choose two values, x_{left} and x_{right}, with $x_{left} < x_{right}$, such that $f(x_{left})f(x_{right}) < 0$. There must be a value of x such that $f(x) = 0$ in the interval $[x_{left}, x_{right}]$.
2. Choose the midpoint, $x_{mid} = x_{left} + \frac{1}{2}(x_{right} - x_{left}) = \frac{1}{2}(x_{right} + x_{left})$, as the guess for x.
3. If $f(x_{mid})$ has the same sign as $f(x_{left})$, then replace x_{left} by x_{mid}; otherwise, replace x_{right} by x_{mid}. Thus, we halved the interval for the location of the root.
4. Repeat steps 2 and 3 until the desired level of precision is achieved.

Bisection method - error

$$
\begin{aligned}
|x - x_{mid}| &\leq x_{mid} - x_{left} = x_{right} - x_{mid} \\
&= \frac{1}{2}(x_{right} - x_{left}) = \cdots = \frac{1}{2^n}(b-a)
\end{aligned}
$$

$$
|x - x_{mid}^n| \leq \frac{1}{2^n}(b-a) \leq \epsilon
$$

$$
n \geq \frac{\log((b-a)/\epsilon)}{log2}
$$

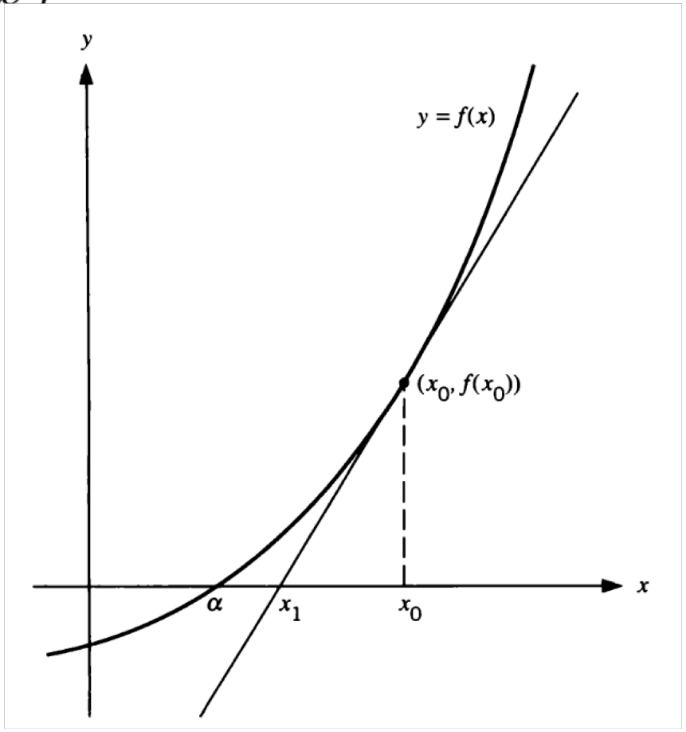
- At each iteration the error is reduced by 1/2

Newton-Raphson method

$$0 = f(x^*) \approx f(x) + (x^* - x) f'(x)$$

$$\Rightarrow \quad x^* = x - \frac{f(x)}{f'(x)}$$

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



- Can converge very fast
- Needs accurate starting point
- Needs both the function and its derivative

Newton-Raphson method - examples

Example 1: $f(x) = x^6 - x - 1, f'(x) = 6x^5 - 1.$

n	x_n	$f(x_n)$	$x_n - x_{n-1}$
0	1.5	8.89E+1	
1	1.30049088	2.54E+1	-2.00E-1
2	1.18148042	5.38E-1	-1.19E-1
3	1.13945559	4.92E-2	-4.20E-2
4	1.13477763	5.50E-4	-4.68E-3
5	1.13472415	7.11E-8	-5.35E-5
6	1.13472414	1.55E-15	-6.91E-9

Example 2: $f(x) = x^2 + 1, f'(x) = 2x$

n	x_n	$f(x_n)$	$x_n - x_{n-1}$
0	0.57735027	1.3333	
1	-0.57735027	1.3333	-1.1547
2	0.57735027	1.3333	1.1547
3	-0.57735027	1.3333	-1.1547

Newton-Raphson method – error estimate

$$\epsilon_n = x^* - x_n \qquad \Rightarrow \qquad \epsilon_{n+1} = \epsilon_n + \frac{f(x_n)}{f'(x_n)}$$

Using the Taylor expansion:

$$0 = f(x^*) = f(x_n) + (x^* - x_n) f'(x_n) + \frac{(x^* - x_n)^2}{2!} f''(x_n) + \cdots$$

$$\Rightarrow \quad \frac{f(x_n)}{f'(x_n)} = -\epsilon_n - \frac{\epsilon_n^2 f''(x_n)}{2 f'(x_n)}$$

Finally: $\boxed{\epsilon_{n+1} = -\frac{\epsilon_n^2 f''(x_n)}{2 f'(x_n)}}$

Rate of convergence

$$|x^* - x_{n+1}| \le c|x^* - x_n|^p, \qquad n \ge 0$$

for some constant $c \ge 0$.

1. *Linear convergence:* $p = 1$, $c <?$

   e.g., Bisection method.

2. *Quadratic convergence:* $p = 2$.

   e.g., Newton-Raphson method.

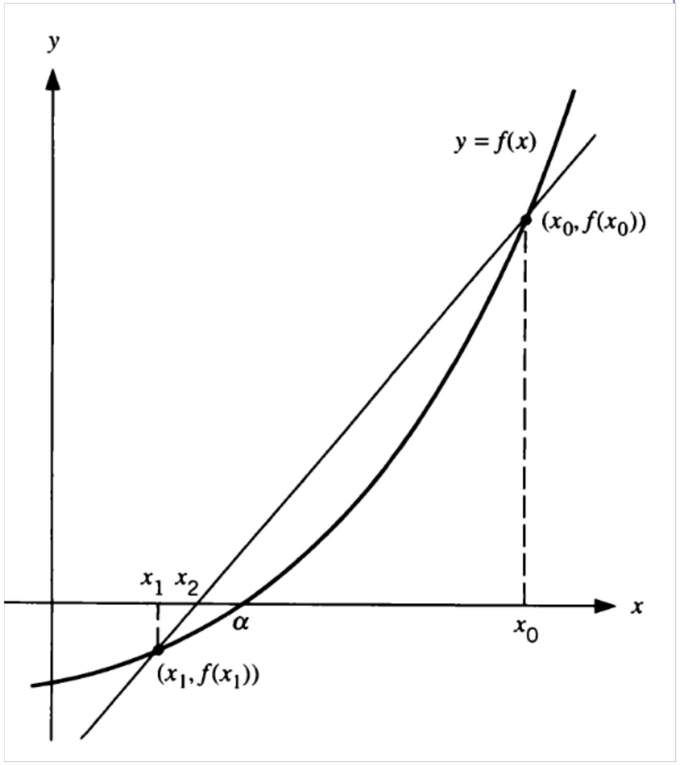
The secant method

Suppose the derivative is not available:

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

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

$$\begin{aligned} x_{n+1} &= x_n - \frac{f(x_n)}{f'(x_n)} \\ &\approx x_n - f(x_n) \frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} \end{aligned}$$



Secant method - rate of convergence

Example 1: $f(x) = x^6 - x - 1, x_0 = 2.0, x_1 = 1.0$

n	x_n	$f(x_n)$	$x_n - x_{n-1}$
2	1.01612903	-9.15E-1	1.61E-2
3	1.19057777	6.57E-2	1.74E-1
4	1.11765583	-1.68E-1	-7.29E-2
5	1.13253155	-2.24E-2	1.49E-2
6	1.13481681	9.54E-4	2.29E-3
7	1.13472365	-5.07E-6	-9.32E-5
8	1.13472414	-1.13E-8	4.92E-7

Newton method

2	1.18148042
3	1.13945559
4	1.13477763
5	1.13472415
6	1.13472414

Rate of convergence $p = (\sqrt{5} + 1)/2 = 1.62$

Hybrid methods

Bisection+Newton (stability+rapid convergence)

$$a \leq \tilde{r} = r - \frac{f(r)}{f'(r)} \leq b$$

$$\Rightarrow 0 \leq (r-a)f'(r) - f(r) = A(r)$$

$$0 \geq (r-b)f'(r) - f(r) = B(r) \, .$$

Thus, if $A(r) \times B(r) \leq 0$, Newton-Raphson.

if $A(r) \times B(r) > 0$, Bisection.

Alternatively, just calculate $(\tilde{r} - a) \times (\tilde{r} - b)$.

If derivative is not available: Bisection+secant

Accelerated method

- If function is computationally expensive, we should try not discard information!
- Newton method uses 1 point, while bisection, secant use 2 points. What about **using 3 points**?

Polynomial approx:

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

$$c = f(x_2),$$

$$b = \frac{(x_0 - x_2)^2[f(x_1) - f(x_2)] - (x_1 - x_2)^2[f(x_0) - f(x_2)]}{(x_0 - x_1)(x_0 - x_2)(x_1 - x_2)},$$

$$a = \frac{(x_1 - x_2)[f(x_0) - f(x_2)] - (x_0 - x_2)[f(x_1) - f(x_2)]}{(x_0 - x_1)(x_0 - x_2)(x_1 - x_2)}.$$

Accelerated method

$$f(x) \approx p(x) = a_2(x-x_2)^2 + a_1(x-x_2) + a_0$$

New estimate of the root: $x_3 - x_2 = \dfrac{-a_1 \pm \sqrt{a_1^2 - 4a_2a_0}}{2a_2}$

with which sign?

$$x_3 = x_2 - \frac{2a_0}{a_1 + \sqrt{a_1^2 - 4a_2a_0}}, \qquad a_1 \geq 0 \ .$$

$$x_3 = x_2 - \frac{2a_0}{a_1 - \sqrt{a_1^2 - 4a_2a_0}}, \qquad a_1 \leq 0 \ .$$

It is *robust, virtually failsafe, and no derivatives.*

see book of DeVries for extended discussion

General theory of one-point iteration

$$f(x) = 0 \quad \Rightarrow \quad x = G(x)$$
$$\Rightarrow \quad x_{n+1} = G(x_n)$$

REMARK: the Newton method is of this type

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

Here we only touch the main points of this general problem see the book of Atkinson & Han for details

One-point iteration - examples

$$f(x) = x^2 - 5 = 0,\ x = \pm\sqrt{5} = \pm 2.2361$$

$$(I1) \quad x_{n+1} = 5 + x_n - x_n^2 \qquad (I3) \quad x_{n+1} = 1 + x_n - \frac{1}{5}x_n^2$$

$$(I2) \quad x_{n+1} = 5/x_n \qquad (I4) \quad x_{n+1} = \frac{1}{2}\left(x_n + \frac{5}{x_n}\right)$$

Start from $x_0 = 2.5$,

n	$x_n(I1)$	$x_n(I2)$	$x_n(I3)$	$x_n(I4)$
0	2.5	2.5	2.5	2.5
1	1.25	2.0	2.25	2.25
2	4.6875	2.5	2.2375	2.2361
3	-12.2852	2.0	2.2362	2.2361
$G'(\sqrt{5})$	$1-2\sqrt{5}$	-1.0	$1-\frac{2}{5}\sqrt{5}$	0

Why this behavior? Discuss on blackboard…

Formal properties - 1

1. Let $G(x)$ be a continuous function for an interval $[a, b]$, and suppose G satisfies the property

$$a \leq x \leq b \Rightarrow a \leq G(x) \leq b \; . \tag{25}$$

Then the equation $x = G(x)$ has at least one solution x^* in the interval $[a, b]$.

Intuitive (make drawing)

For detailed proof: see the textbook or Prof Lin's note

Formal properties - 2

2. Assume $G(x)$ and $G'(x)$ are continuous for $[a,b]$, and assume G satisfies Eq. (25). Further assume that $\lambda \equiv \text{Maximum}_{a \le x \le b} |G'(x)| < 1$. Then

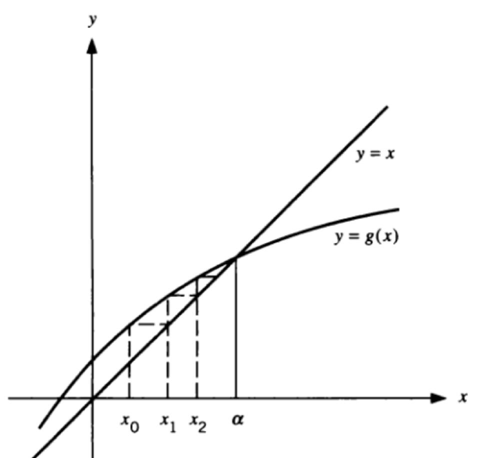
   (a) There is a unique solution x^* of $x = G(x)$ in the interval $[a,b]$.

   (b) For any initial estimate x_0 in $[a,b]$, the iterates x_n will converge to x^*.

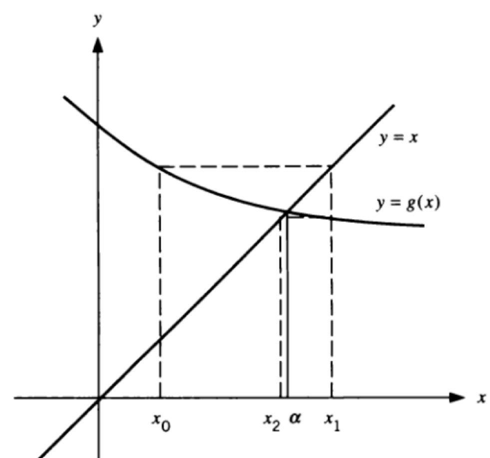
   (c) $$|x^* - x_n| \le \frac{\lambda^n}{1-\lambda}|x_0 - x_1|, \quad n \ge 0 \ . \tag{26}$$

   (d) $$Lim_{n\to\infty} \frac{x^* - x_{n+1}}{x^* - x_n} = G'(x^*) \ . \tag{27}$$

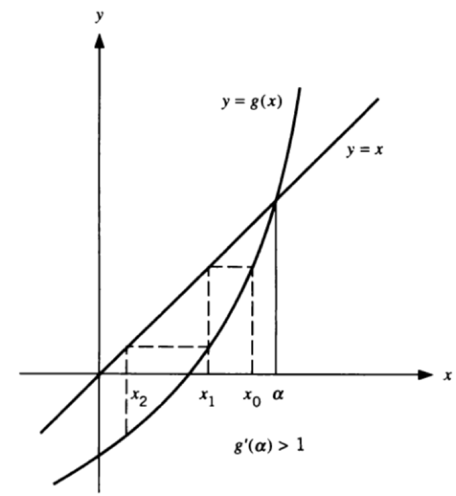
Graphical examples



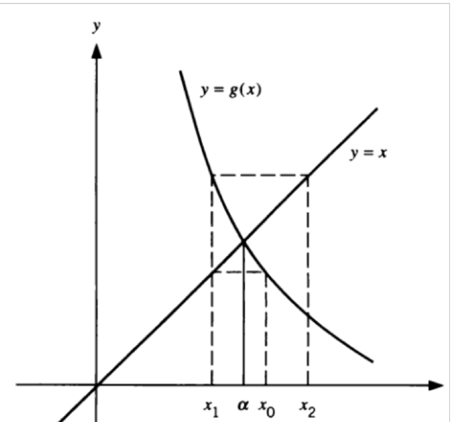
$0 < g'(\alpha) < 1$



$-1 < g'(\alpha) < 0$



$g'(\alpha) > 1$



$g'(\alpha) < -1$

Question: derivative of G(x) for the Newton-Raphson method?

Aitken's estimate of the error

Use property (d): $$x^* - x_n \approx \lambda(x^* - x_{n-1})$$

This gives the error: $$\boxed{x^* - x_n \approx \frac{\lambda_n}{1-\lambda_n}(x_n - x_{n-1})}$$

How to estimate λ? $$\lambda_n = \frac{x_n - x_{n-1}}{x_{n-1} - x_{n-2}}$$

Justification: $$\lambda_n = \frac{G(x_{n-1}) - G(x_{n-2})}{x_{n-1} - x_{n-2}} = G'(c_n)$$

Difficult situations – multiple roots

- Multiple roots $f(x) = (x-a)^m h(x)$

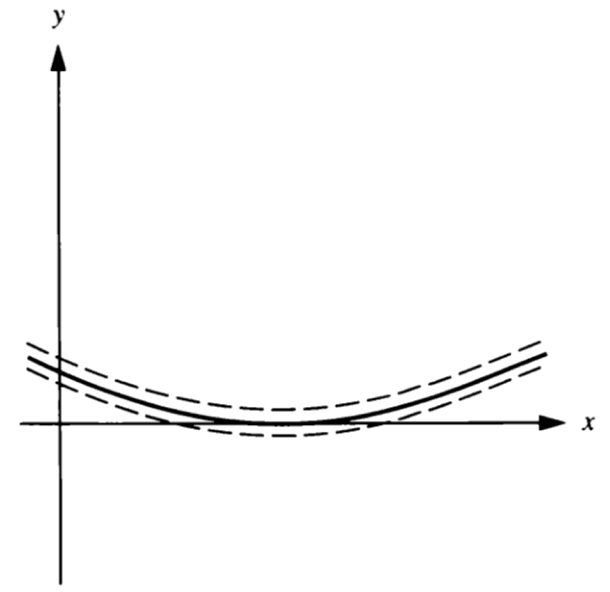
Slower convergence & noise in evaluation of $f(x)$

$f(x) = (x-1.1)^3(x-2.1)$

n	x_n	$f(x_n)$	$x^* - x_n$	Ratio
0	0.800000	0.03510	0.300000	
1	0.892857	0.01073	0.207143	0.690
2	0.958176	0.00325	0.141824	0.685
3	1.00344	0.00099	0.09656	0.681
4	1.03486	0.00029	0.06514	0.675
5	1.05581	0.00009	0.04419	0.678
6	1.07028	0.00003	0.02972	0.673
7	1.08092	0.00000	0.01908	0.642

Thus, with any root of multiplicity $m \geq 2$, the

Bisection method is always better!



Double root

Difficult situations – multiple roots

- Multiple roots $f(x) = (x-a)^m h(x)$

Slower convergence & noise in evaluation of $f(x)$

$$\frac{x^* - x_n}{x^* - x_{n-1}} \to \lambda = \frac{m-1}{m}$$

One can use the ratio to estimate *m*

Try to remove multiple root, e.g., $F(x) = f^{(m-1)}(x)$

Difficult situations – unstable problems

$$
\begin{aligned}
f(x) &= (x-1)(x-2)(x-3)(x-4)(x-5)(x-6)(x-7) \\
&= x^7 - 28x^6 + \cdots \\
F(x) &= x^7 - 28.002x^6 + \cdots
\end{aligned}
$$

Root of f(x)	Root of F(x)
1	1.0000028
2	1.9989382
3	3.0331253
4	3.8195692
5	5.4586758 + 0.54012578 i
6	5.4586758 - 0.54012578 i
7	7.2330128

High precision arithmetic? Reformulate the problem?

Other issues

- How to find all the roots?

No simple method: needs some insight on the particular function, or scan the desired interval.

- Multi-dimensional functions?

- Other methods?

See also Chapter 9 of *Numerical Recipes*

Summary

- Simple algorithms: Bisection, Newton, Secant
- Rate of convergence, stability
- Hybrid methods, three-point iteration
- General properties of one-point iterations
- Difficulties