chapter 2 : root-finding

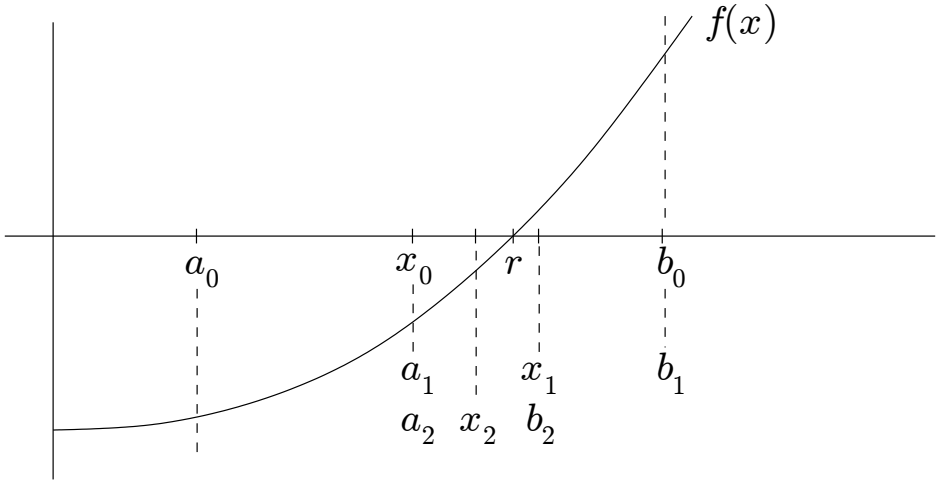
def : Given a function $f(x)$, a root is a number r satisfying $f(r) = 0$.

ex : $f(x) = x^2 - 3 \;\Rightarrow\; r = \pm\sqrt{3}$

question : How can we find the roots of a general function $f(x)$?

2.1 bisection method

idea : Find an interval $[a, b]$ such that $f(a)$ and $f(b)$ have opposite sign. Then $f(x)$ has a root in $[a, b]$ (Intermediate Value Theorem, Math 451 - advanced calculus).



Consider the midpoint $x_0 = \frac{1}{2}(a + b)$. The root r is contained in either the left subinterval or the right subinterval; to determine which one, compute $f(x_0)$. Then repeat.

ex : $f(x) = x^2 - 3$, $f(1) = -2$, $f(2) = 1 \Rightarrow f(x)$ has a root in $[1, 2]$, $r = 1.73205$

n	a_n	b_n	x_n	$f(x_n)$	$\lvert r - x_n \rvert$
0	1	2	1.5	-0.75	0.2321
1	1.5	2	1.75	0.0625	0.0179
2	1.5	1.75	1.625	-0.3594	0.1071
3	1.625	1.75	1.6875	-0.1523	0.0446

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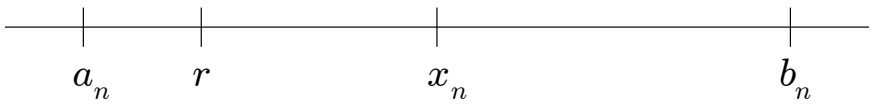
bisection method (assume $f(a) \cdot f(b) < 0$)

1. $n = 0$, $a_0 = a$, $b_0 = b$
2. $x_n = \frac{1}{2}(a_n + b_n)$: current estimate of the root
3. if $f(x_n) \cdot f(a_n) < 0$, then $a_{n+1} = a_n$, $b_{n+1} = x_n$
4. else $a_{n+1} = x_n$, $b_{n+1} = b_n$
5. set $n = n + 1$ and go to line 2

stopping criterion : here are three options

$|b_n - a_n| < \epsilon$, $|f(x_n)| < \epsilon$, $n = n_{\max}$

error bound



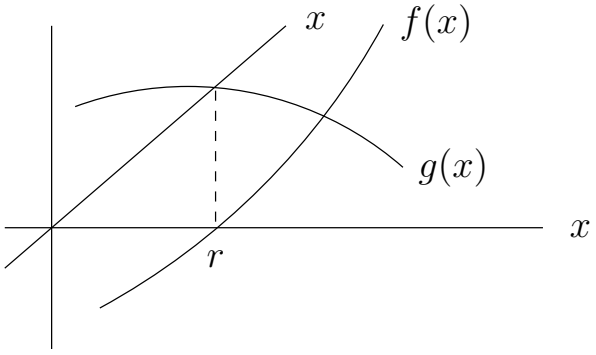
$|r - x_n| \le \frac{1}{2}|b_n - a_n| = (\frac{1}{2})^2|b_{n-1} - a_{n-1}| = \cdots = (\frac{1}{2})^{(n+1)}|b_0 - a_0|$

ex : how many steps are needed to ensure that the error is less than 10^{-3} ?

$[a, b] = [1, 2]$, $|r - x_n| \le (\frac{1}{2})^{(n+1)}|b_0 - a_0| \le 10^{-3} \Rightarrow n + 1 \ge 10 \Rightarrow n \ge 9$

2.3 fixed-point iteration

Suppose $f(x) = 0$ is equivalent to $x = g(x)$. Then r is a root of $f(x)$ if and only if r is a fixed point of $g(x)$.



We try to solve $x = g(x)$ by computing $x_{n+1} = g(x_n)$ with some initial guess x_0. This is called fixed-point iteration.

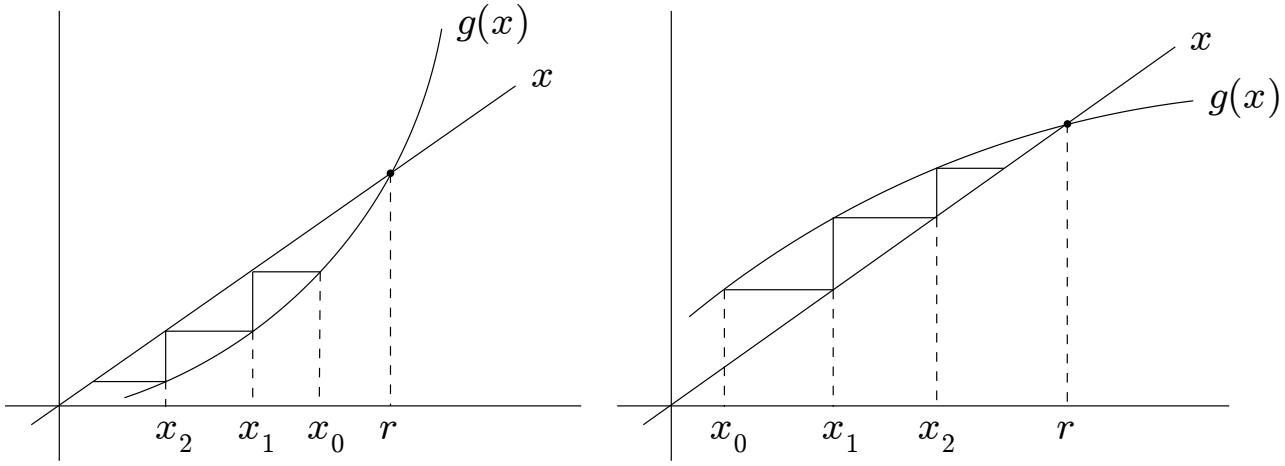
ex : $f(x) = x^2 - 3 = 0$

$x = g_1(x) = \dfrac{3}{x}$, $x = g_2(x) = x - (x^2 - 3)$, $x = g_3(x) = x - \frac{1}{2}(x^2 - 3)$

	case 1	case 2	case 3
n	x_n	x_n	x_n
0	1.5	1.5	1.5
1	2	2.25	1.875
2	1.5	0.1875	1.6172
3	2	3.1523	1.8095
4	1.5	-3.7849	1.6723
5	2	-15.1106	1.7740

$\Rightarrow$ Case 1 and case 2 diverge,
but case 3 converges (recall : $r = 1.73205$).

question : what determines whether fixed-point iteration converges or diverges? Consider two examples.



The 1st example diverges and the 2nd example converges.

thm

Assume that x_0 is sufficiently close to r and let $k = |g'(r)|$. Then fixed-point iteration converges if and only if $k < 1$.

note : This is consistent with the two examples above.

pf (idea)

$|r - x_{n+1}| = |g(r) - g(x_n)| \sim |g'(r)| \cdot |r - x_n|$

Taylor expansion : $g(x_n) = g(r) + g'(r)(x_n - r) + \cdots$

$|r - x_{n+1}| \sim k|r - x_n| \sim k^2|r - x_{n-1}| \sim \cdots \sim k^{n+1}|r - x_0|$ ok

note

1. We showed that $|r - x_{n+1}| \sim k|r - x_n|$. This is called linear convergence and k is called the asymptotic error constant.

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recall : $f(x) = x^2 - 3$, $r = \sqrt{3} = 1.73205$

$g_1(x) = \dfrac{3}{x} \Rightarrow g_1'(x) = -\dfrac{3}{x^2} \Rightarrow k = |g_1'(r)| = 1$: diverges

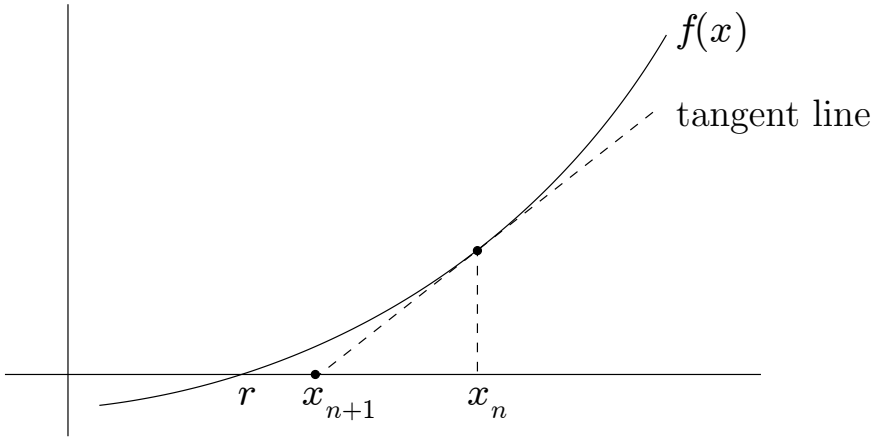
$g_2(x) = x - (x^2 - 3) \Rightarrow g_2'(x) = 1 - 2x \Rightarrow k = |g_2'(r)| = 2.4641$: diverges

$g_3(x) = x - \frac{1}{2}(x^2 - 3) \Rightarrow g_3'(x) = 1 - x \Rightarrow k = |g_3'(r)| = 0.73205$: converges

2. The bisection method also converges linearly, with $k = \frac{1}{2}$.

2.3 Newton's method

idea : local linear approximation



$$\text{slope} = f'(x_n) = \frac{0 - f(x_n)}{x_{n+1} - x_n} \;\Rightarrow\; x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

ex

$$f(x) = x^2 - 3 \;\Rightarrow\; x_{n+1} = x_n - \frac{x_n^2 - 3}{2x_n}$$

n	x_n	$f(x_n)$	$\lvert r - x_n\rvert$
0	1.5	-0.75	0.23205081
1	1.75	0.0625	0.01794919
2	1.73214286	0.00031888	0.00009205

: rapid convergence

note

Newton's method is an example of fixed point iteration, $x_{n+1} = g(x_n)$, where the iteration function is $g(x) = x - \dfrac{f(x)}{f'(x)}$.

$$g'(x) = 1 - \frac{f'(x)^2 - f(x)\cdot f''(x)}{f'(x)^2} \;\Rightarrow\; g'(r) = 1 - \frac{f'(r)^2 - f(r)\cdot f''(r)}{f'(r)^2} = 0$$

This implies that Newton's method converges faster than linearly; in fact it can be shown that $|r - x_{n+1}| \le C|r - x_n|^2$, i.e. quadratic convergence.

pf

$$r - x_{n+1} = g(r) - g(x_n) = \cancel{g(r)} - \big(\cancel{g(r)} + \cancel{g'(r)}(x_n - r) + O((x_n - r)^2)\big) \quad \text{ok}$$

ex : equation of state of chlorine gas

ideal gas law : $PV = nRT$, P : pressure , V : volume , T : temperature

n : number of moles present

R : universal gas constant , $R = 0.08206$ atm $\cdot$ liter/(mole $\cdot$ K)

van der Waals equation : $\left(P + \frac{n^2 a}{V^2}\right)(V - nb) = nRT$

$a = 6.29$ atm $\cdot$ liter^2/mole^2 (accounts for intermolecular attractive forces)

$b = 0.0562$ liter/mole (accounts for size of gas molecules)

Take $n = 1$ mole, $P = 2$ atm, $T = 313$ K, and find V by Newton's method with starting guess V_0 given by the ideal gas law.

$$f(V) = \left(P + \frac{n^2 a}{V^2}\right)(V - nb) - nRT \ , \ f'(V) = \left(P + \frac{n^2 a}{V^2}\right) + \left(\frac{-2n^2 a}{V^3}\right)(V - nb)$$

n	V_n
0	12.84238 99999 99980
1	12.65115 48134 06302
2	12.65109 93371 19016 $\approx$ 0.2 atm less than V_0 given by ideal gas law

We infer that V_0 has 2 correct digits and V_1 has 5 correct digits. How many correct digits does V_2 have? (hw)

summary

method	rate of convergence	cost per step
bisection	linear , $k = \frac{1}{2}$	$f(x_n)$
fixed-point iteration	linear , $k = \lvert g'(r)\rvert$	$g(x_n)$
Newton	quadratic	$f(x_n), f'(x_n)$

note : Bisection is guaranteed to converge if the initial interval contains a root; the other methods are sensitive to the choice of x_0.

root-finding for nonlinear systems

ex : chemical reactions

$\left.\begin{array}{r} 2A + B \rightleftharpoons C \\ A + D \rightleftharpoons C \end{array}\right\}$: reversible reactions for reactants A, B, D and product C

a_0, b_0, d_0 : initial concentrations (moles/liter) in chemical reactor (known)

c_1, c_2 : equilibrium concentrations of C produced by each reaction (unknown)

k_1, k_2 : equilibrium reaction constants (known)

These variables are related by the law of mass action.

$$\frac{c_1 + c_2}{(a_0 - 2c_1 - c_2)^2(b_0 - c_1)} = k_1$$

$$\frac{c_1 + c_2}{(a_0 - 2c_1 - c_2)(d_0 - c_2)} = k_2$$

Hence to find c_1, c_2 we need to solve a system of nonlinear equations with 2 equations and 2 unknowns.

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Newton's method for nonlinear systems

First note the following alternative derivation of Newton's method for the case of 1 equation and 1 unknown, $f(x) = 0$.

$$\cancelto{0}{f(x_{n+1})} = f(x_n) + f'(x_n)(x_{n+1} - x_n) + \cancelto{0}{\cdots\cdots} \Rightarrow x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Now consider a system of 2 equations and 2 unknowns.

$f(x, y) = 0\ ,\ g(x, y) = 0$

Given (x_n, y_n), we want to find (x_{n+1}, y_{n+1}).

$$\begin{aligned} \cancelto{0}{f(x_{n+1}, y_{n+1})} &= f(x_n, y_n) + \frac{\partial f}{\partial x}(x_n, y_n)(x_{n+1} - x_n) \\ &\quad + \frac{\partial f}{\partial y}(x_n, y_n)(y_{n+1} - y_n) + \cancelto{0}{\cdots\cdots} \\ \cancelto{0}{g(x_{n+1}, y_{n+1})} &= g(x_n, y_n) + \frac{\partial g}{\partial x}(x_n, y_n)(x_{n+1} - x_n) \\ &\quad + \frac{\partial g}{\partial y}(x_n, y_n)(y_{n+1} - y_n) + \cancelto{0}{\cdots\cdots} \end{aligned}$$

$$\Rightarrow \begin{pmatrix} f_x & f_y \\ g_x & g_y \end{pmatrix}\Big|_{(x_n, y_n)} \cdot \begin{pmatrix} x_{n+1} - x_n \\ y_{n+1} - y_n \end{pmatrix} = \begin{pmatrix} -f(x_n, y_n) \\ -g(x_n, y_n) \end{pmatrix}$$

↑
Jacobian matrix

note

1. Given (x_n, y_n), we can solve for (x_{n+1}, y_{n+1}). Each step has the form $Ax = b$, where A is a given matrix, b is a given vector, and we must solve for the vector x.

2. hw3 has an application to the chemical reaction system