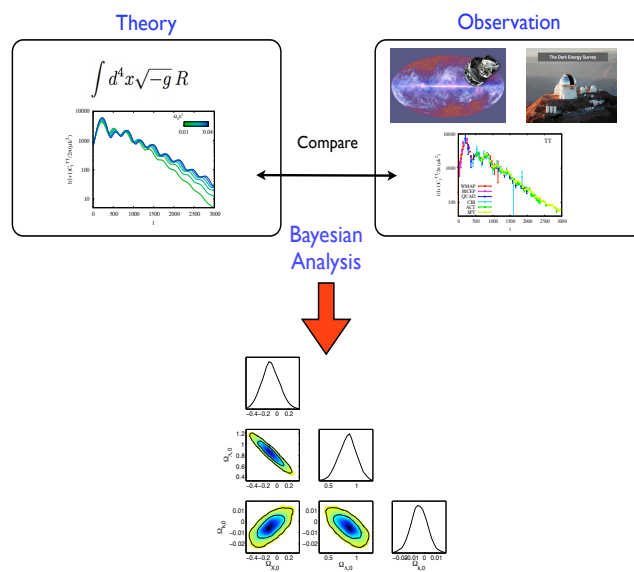


Numerical Methods



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1

Roots of equations

Although there were equations like this that could be solved directly, there were many more that could not. For example, even an apparently simple function such as $f(x) = e^x - x$ cannot be solved analytically. In such instances, the only alternative is an approximate solution technique.

By definition, a function given by $y = f(x)$ is **algebraic** if it can be expressed in the form

$$f_n y^n + f_{n-1} y^{n-1} + \dots + f_1 y + f_0 = 0 \quad (1.1)$$

where $f_i =$ an i th-order polynomial in x . **Polynomials** are a simple class of algebraic functions.

A **transcendental** function is one that is nonalgebraic. These include trigonometric, exponential, logarithmic, and other, less familiar, functions.

$$f(x) = \ln x^2 - 1.$$

1.1 Graphical Methods

To make a plot of the function and observe where it crosses the x axis.

Graphical techniques are of limited practical value because they are not precise. However, graphical methods can be utilized to obtain rough estimates of roots. (py: roots, sin)

1. ROOTS OF EQUATIONS

1.2 Bracketing Methods

For a function that typically changes sign in the vicinity of a root. These techniques are called bracketing methods because two initial guesses for the root are required.

1.3 The Bisection Method

Alternatively called binary chopping, interval halving, or **Bolzano's method**. Is a search method in which the interval is always divided in half.

Suppose f is a continuous function defined on the interval $[a, b]$, with $f(a)$ and $f(b)$ of opposite sign:

$$f(a)f(b) < 0$$

By the Intermediate Value Theorem, there exists a number p in (a, b) with $f(p) = 0$. We assume, for simplicity that the root in this interval is unique.

1. Find middle point $c = (a + b)/2$.
2. If $f(c) == 0$, then c is the root of the solution.
3. Else $f(c) \neq 0$
 - (a) If value $f(a) * f(c) < 0$ then root lies between a and c . So we recur for a and c
 - (b) Else If $f(b) * f(c) < 0$ then root lies between b and c . So we recur b and c .
 - (c) Else given function doesn't follow one of assumptions.

INPUT: endpoints a, b ; tolerance TOL ; maximum number of iterations N_0

To start the Bisection algorithm, an interval $[a, b]$ must be found with $f(a)f(b) < 0$. At each step the length of the interval known to contain a zero of f is reduced by a factor of 2; hence it is advantageous to choose the initial interval as small as possible.

improvement: For $f(x) = 2x^3 - x^2 + x - 1$. Starting on $[0, 1]$ instead of $[-4, 4]$ will reduce by 3 the number of iterations required to achieve a specified accuracy.

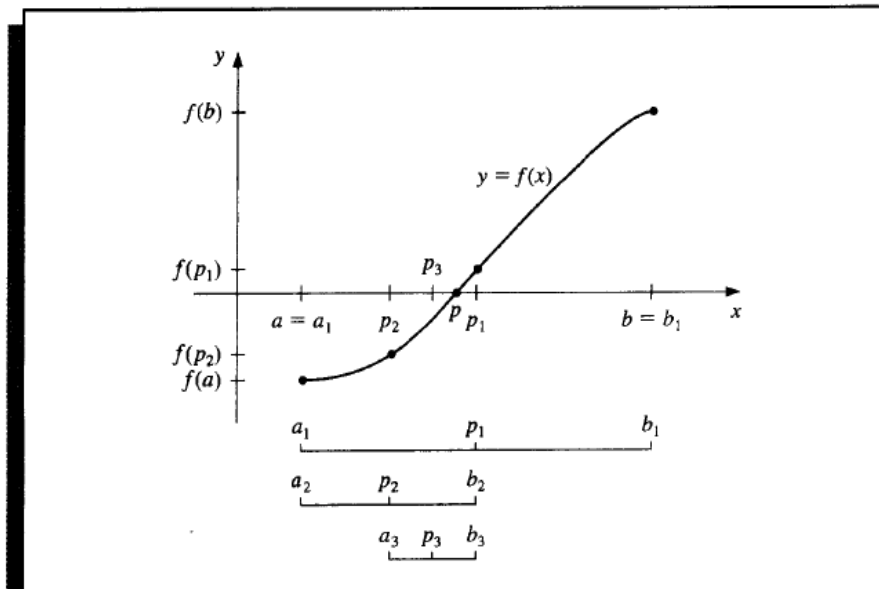
Step 1: Choose lower x_l and upper x_u guesses for the root such that the function changes sign over the interval. This can be checked by ensuring that $f(x_l)f(x_u) < 0$.

Step 2: An estimate of the root x_r is determined by

$$x_r = \frac{x_l + x_u}{2}$$

Step 3: Make the following evaluations to determine in which subinterval the root lies:

- (a) If $f(x_l)f(x_r) < 0$, the root lies in the lower subinterval. Therefore, set $x_u = x_r$ and return to step 2.
- (b) If $f(x_l)f(x_r) > 0$, the root lies in the upper subinterval. Therefore, set $x_l = x_r$ and return to step 2.
- (c) If $f(x_l)f(x_r) = 0$, the root equals x_r ; terminate the computation.



$$|p_N - p_{N-1}| < \epsilon,$$

$$\frac{|p_N - p_{N-1}|}{|p_N|} < \epsilon, \quad p_N \neq 0, \quad \text{or}$$

$$|f(p_N)| < \epsilon.$$

Figure 1.1: Summary of the numerical methods covered in this course.

1.3.1 Termination criteria

Consider the equation $f(x) = x^3 + 4x^2 - 10 = 0$ has a root in $[1, 2]$.

Theorem: Suppose that $f \in C[a, b]$ and $f(a)f(b) < 0$. The Bisection method generates a

1. ROOTS OF EQUATIONS

sequence $\{p_n\}_{n=1}^{\infty}$ approximating a zero p of f with

$$|p_n - p| \leq \frac{b-a}{2^n}, \quad \text{when } n \geq 1. \quad (1.2)$$

(py: exercise) (hw: determine de number of iterations necessary to solve $f(x) = x^3 + 4x^2 - 10 = 0$ with accuracy 10^{-3} - using the code and the theorem.) (hw: same with $f(x) = \ln x^2 - 1$. on the interval $[0.1, 5]$).

n	a_n	b_n	p_n	$f(p_n)$
1	1.0	2.0	1.5	2.375
2	1.0	1.5	1.25	-1.79687
3	1.25	1.5	1.375	0.16211
4	1.25	1.375	1.3125	-0.84839
5	1.3125	1.375	1.34375	-0.35098
6	1.34375	1.375	1.359375	-0.09641
7	1.359375	1.375	1.3671875	0.03236
8	1.359375	1.3671875	1.36328125	-0.03215
9	1.36328125	1.3671875	1.365234375	0.000072
10	1.36328125	1.365234375	1.364257813	-0.01605
11	1.364257813	1.365234375	1.364746094	-0.00799
12	1.364746094	1.365234375	1.364990235	-0.00396
13	1.364990235	1.365234375	1.365112305	-0.00194

To determine which subinterval of $[a_n, b_n]$ contains a root of f , it is better to make use of the *signum* function. The test

$$\text{sign}(f(a_n))\text{sign}(f(p_n)) < 0 \quad \text{instead of} \quad f(a_n)f(p_n) < 0 \quad (1.3)$$

gives the same result, but avoids the possibility of overflow or underflow in the multiplication.

The Bisection method, is slow to converge, however it always converges to a solution: thus it is often used as a starter for the more efficient methods.

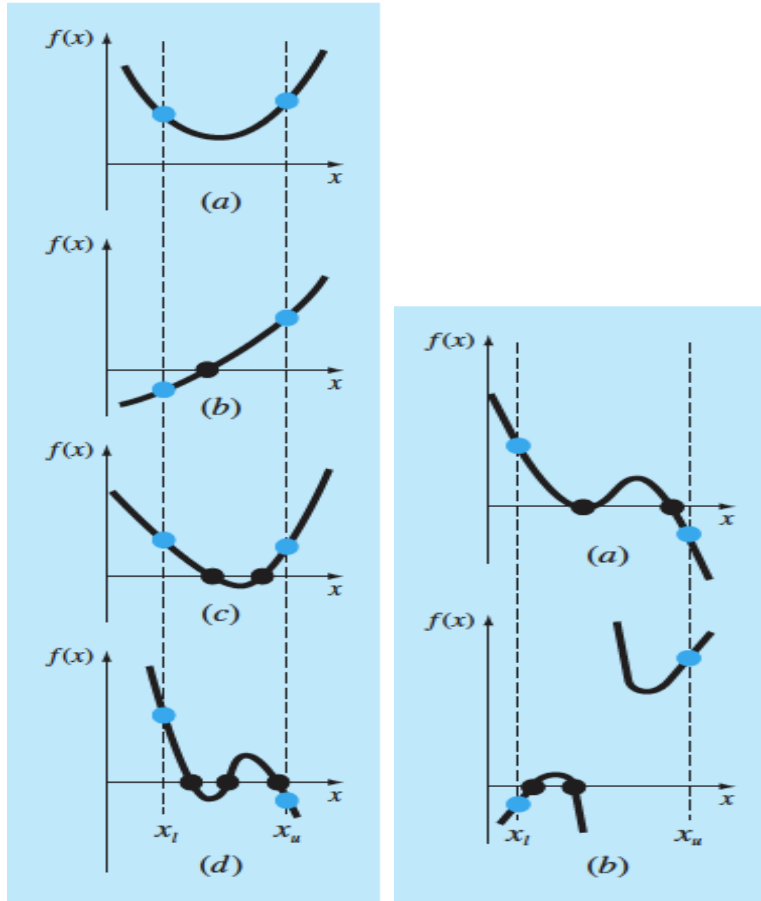


Figure 1.2: Possible Issues when using this method.

1.4 False-Position Method

A **shortcoming** of the bisection method is that, in dividing the interval from a to b into equal halves, no account is taken of the magnitudes of $f(a)$ and $f(b)$. For example, if $f(a)$ is much closer to zero than $f(b)$, it is likely that the root is closer to a than to b .

The intersection of this line with the x axis represents an improved estimate of the root. It is also called the linear interpolation method.

Steps

1. Write equation of the line connecting the two points.

$$y - f(a) = \frac{f(b) - f(a)}{b - a}(x - a) \quad (1.4)$$

1. ROOTS OF EQUATIONS

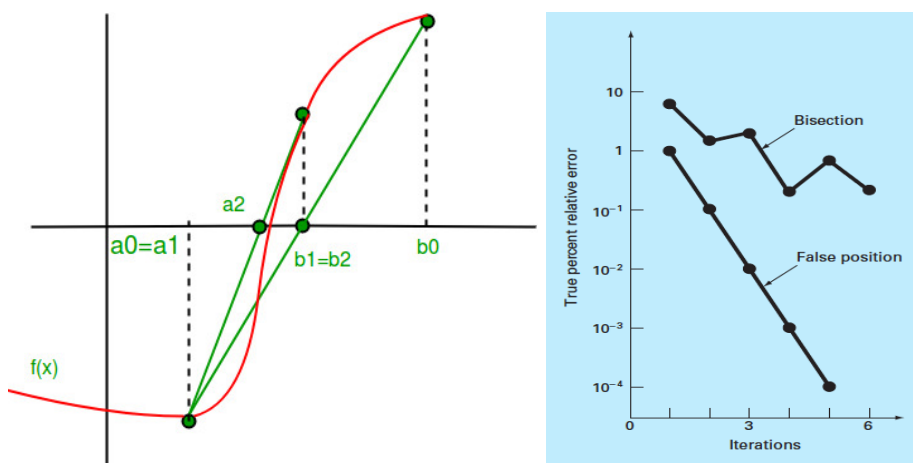
Now we have to find the point which touches x axis. For that we put $y = 0$. So,

$$x = \frac{af(b) - bf(a)}{f(b) - f(a)} \quad (1.5)$$

This will be our c that is $c = x$.

2. If $f(c) = 0$, then c is the root of the solution.
3. Else $f(c) \neq 0$
 - (a) If value $f(a)f(c) < 0$ then root lies between a and c . So we recur for a and c
 - (b) Else If $f(b)f(c) < 0$ then root lies between b and c . So we recur b and c .
 - (c) Else given function doesn't follow one of assumptions.

For the method of false position, one of the initial guesses may stay fixed throughout the computation as the other guess converges on the root.

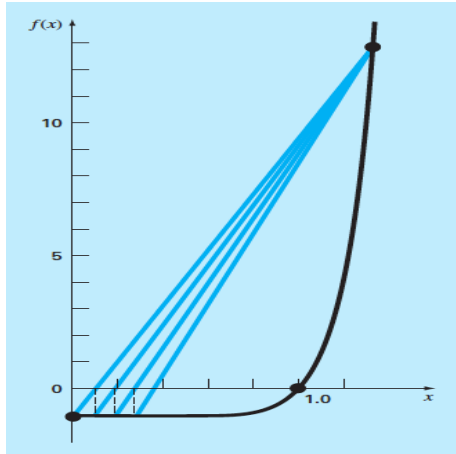


If there's a stuck, then the function value at the stagnant bound can be divided in half. This is called the *modified false position method*.

(hw: how many iterations needed to solve $f(x) = x^{10} - 1$? (39?))

(hw: $5 \sin x^2 - 8 \cos^5 x = 0$ for the root in the interval $[0.5, 1.5]$)

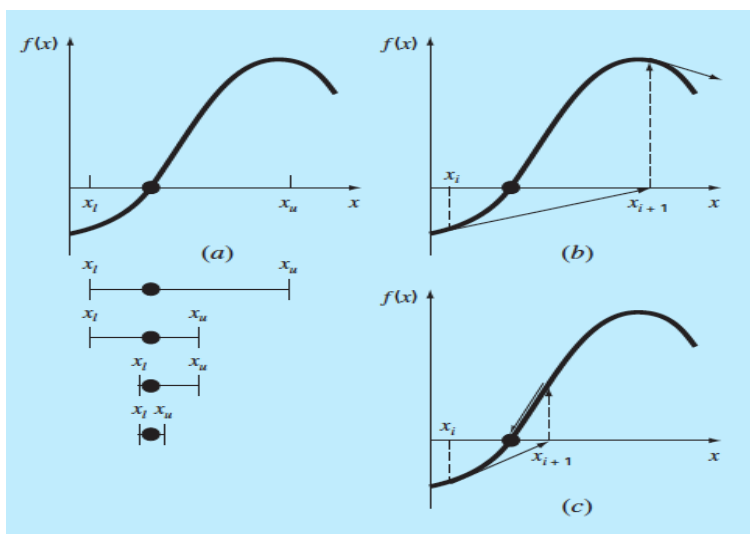
(hw: perform the modified false-position method)



1.5 Open Methods

The bracketing methods are said to be convergent because they move closer to the truth as the computation progresses.

Open methods are based on formulas that require only a single starting value of x (or two starting values) that do not necessarily bracket the root. As such, they sometimes diverge or move away from the true root as the computation progresses. However, when the open methods converge, they usually do so much more quickly than the bracketing methods.



1. ROOTS OF EQUATIONS

1.6 Fixed-Point iteration

A number p is a fixed point for a given function g if $g(p) = p$.

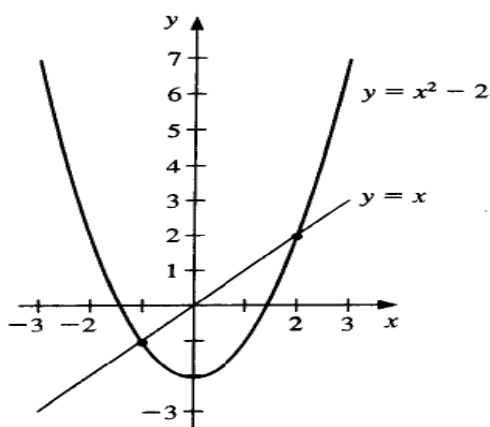
Root finding problems and fixed-point problems are equivalent classes in the following sense. Given a root-finding problem $f(p) = 0$, we can define functions g with a fixed point at p in a number of ways, for example, $g(x) = x - f(x)$. Conversely, if the function g has a fixed point at p , then the function defined by $f(x) = x - g(x)$ has a zero at p .

$$x^2 - 2x + 3 = 0, \quad x = \frac{x^2 + 3}{2} \quad (1.6)$$

Fixed point form is easier to analyze.

(here: find the fix points of $g(x) = x^2 - 2$ for $-2 \leq x \leq 3$) $(-1, 2)$

(py: $f(x) = e^x - x$ roots, same as fixed-point of e^{-x})

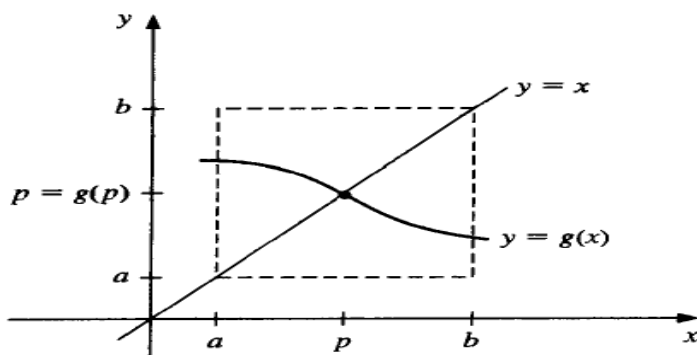


Theorem:

1. If $g \in C[a, b]$ and $g(x) \in [a, b]$ for all $x \in [a, b]$, then g has a fixed point in $[a, b]$.
2. If, in addition, $g'(x)$ exists on (a, b) and a positive constant $k < 1$ exists with

$$|g'(x)| \leq k, \quad \text{for all } x \in (a, b)$$

then the fixed point in $[a, b]$ is unique.



Theorem

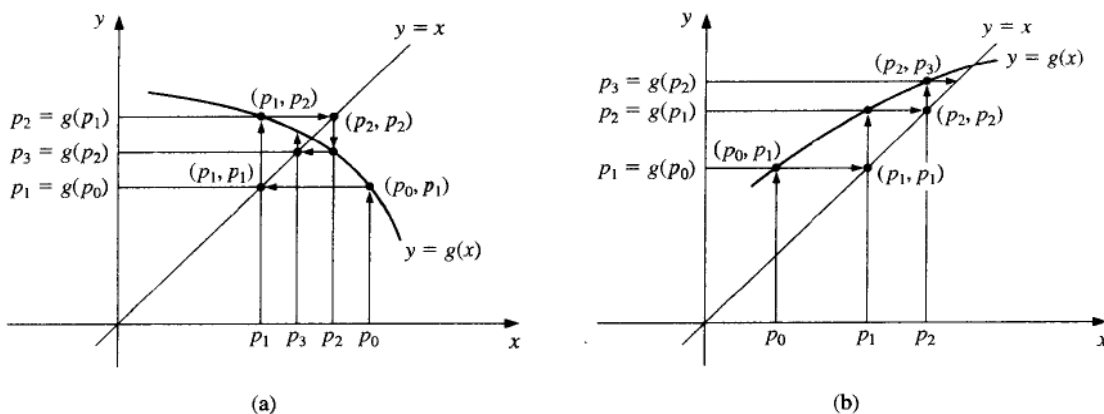
Let $g \in C[a, b]$ be such that $g(x) \in [a, b]$ for all x in $[a, b]$. Suppose, in addition, that g' exists on (a, b) and that a constant $0 < k < 1$ exists with

$$|g'(x)| \leq k \quad \text{for all } x \in (a, b)$$

Then, for any number p_0 in $[a, b]$, the sequence defined by

$$p_n = g(p_{n-1}), \quad n \geq 1$$

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



To approximate the fixed point of a function g , we choose an initial approximation p_0 and generate the sequence $\{p_n\}_{n=0}^{\infty}$ by letting $p_n = g(p_{n-1})$, for each $n \leq 1$. If the sequence converges to p and g is continuous, then p is a solution to $x = g(x)$. Called the fixed-point iteration.

1. ROOTS OF EQUATIONS

(hw: The equation $x^3 + 4x^2 - 10 = 0$ has a unique root in $[1, 2]$. Use... to find the solution 1.365230013 (how many evaluations?))

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

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

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

Corollary: If g satisfies the hypotheses of Theorem, the bounds for the error involved in using p_n to approximate p are given by

$$|p_n - p| \leq \max\{p_0 - a, b - p_0\}$$

and

$$|p_n - p| \leq \frac{k^n}{1-k} |p_1 - p_0|, \quad \text{for all } n \geq 1.$$

1.7 Newton's Method

Newton's (or the Newton-Raphson) method is one of the most powerful and well-known numerical methods for solving a root-finding problem.

Suppose that $f \in C^2[a, b]$. Let $\bar{x} \in [a, b]$ be a approximation to p such that $f'(\bar{x}) \neq 0$ and $|p - \bar{x}|$ is 'small'. Consider the first Taylor polynomial for $f(x)$ expanded about \bar{x} ,

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

Since $f(p) = 0$ and $|p - \bar{x}|$ is small

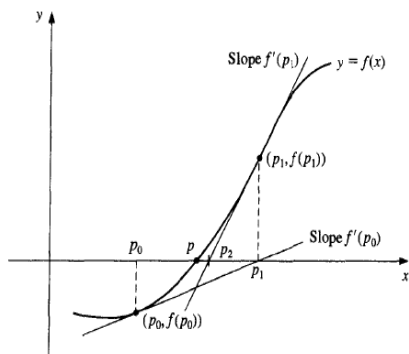
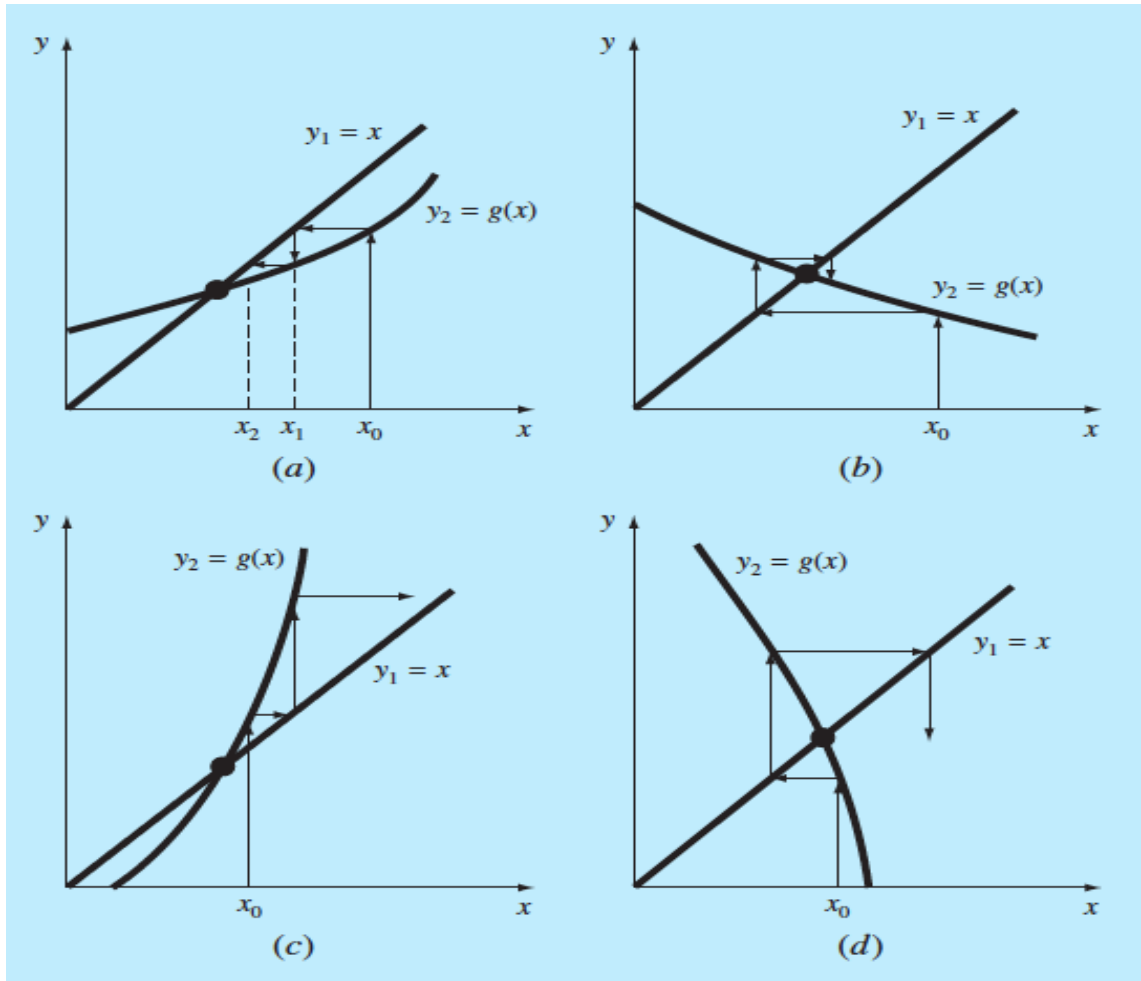
$$0 \approx f(\bar{x}) + (p - \bar{x})f'(\bar{x})$$

Solving for p gives

$$p \approx \bar{x} - \frac{f(\bar{x})}{f'(\bar{x})}.$$

This sets the stage for Newton's method, which starts with an initial approximation p_0 and generates the sequence $\{p_n\}_{n=0}^{\infty}$ by

$$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}, \quad \text{for } n \geq 1.$$



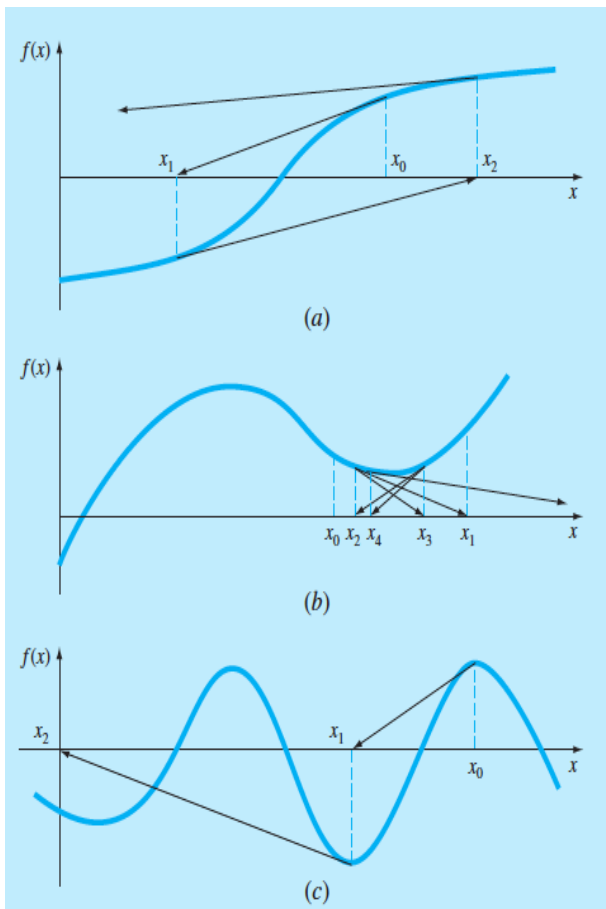
INPUT: initial approximation p_0 ; tolerance TOL; maximum number of iterations N . (py: do it.)

1. ROOTS OF EQUATIONS

1. Compute values of $\text{func}(x)$ and $\text{derivFunc}(x)$ for given initial x
2. Compute h : $h = \text{func}(x) / \text{derivFunc}(x)$
3. While h is greater than allowed error ϵ
 - (a) $h = \text{func}(x) / \text{derivFunc}(x)$
 - (b) $x = x - h$

Pitfalls

Newton Raphson may not converge in some cases. Newton Raphson method requires derivative. Some functions may be difficult to impossible to differentiate. Converges quadratically.



1.8 Secant

By definition

$$f'(p_{n-1}) = \lim_{x \rightarrow p_{n-1}} \frac{f(x) - f(p_{n-1})}{x - p_{n-1}} \quad (1.7)$$

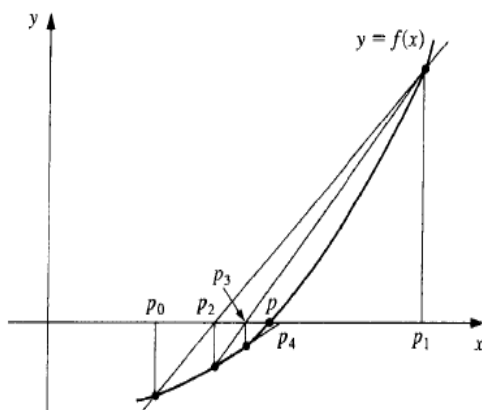
Letting $x = p_{n-2}$ (backward differentiate), we have

$$f'(p_{n-1}) \approx \frac{f(p_{n-2}) - f(p_{n-1})}{p_{n-2} - p_{n-1}} = \frac{f(p_{n-1}) - f(p_{n-2})}{p_{n-1} - p_{n-2}} \quad (1.8)$$

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

$$p_n = p_{n-1} - \frac{f(p_{n-1})(p_{n-1} - p_{n-2})}{f(p_{n-1}) - f(p_{n-2})}$$

This technique is called the secant method. Starting with the two initial approximations p_0 and p_1 (hw: use the secant method and False-position to find a solution $x = \cos x$, $p_0 = 0.5$) (Brent's ?)

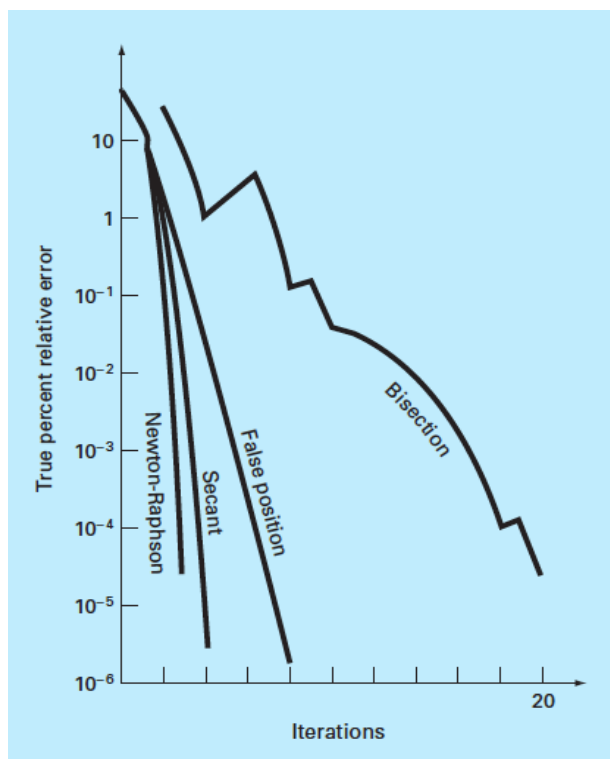


1.9 Multiple Roots

It can be demonstrated that the Newton-Raphson and secant methods are linearly, rather than quadratically, convergent for multiple roots.

(hw: resolver con ambos metodos $f(x) = x^3 - 5x^2 + 7x - 3$)

1. ROOTS OF EQUATIONS



Definition: A solution p of $f(x) = 0$ is a zero of multiplicity m of f if for $x \neq p$, we can write $f(x) = (x - p)^m q(x)$, where $\lim_{x \rightarrow p} q(x) \neq 0$.

Theorem. $f \in C^1[a, b]$ has a simple zero at p in (a, b) if and only if $f(p) = 0$, but $f'(p) \neq 0$.

Theorem. The function $f \in C^m[a, b]$ has a zero of multiplicity m at p in (a, b) if and only if

$$0 = f(p) = f'(p) = f''(p) = \dots = f^{(m-1)}(p), \quad \text{but } f^{(m)}(p) \neq 0.$$

Consider $f(x) = e^x - x - 1$. Since $f(0) = 0$ and $f'(0) = 0$, but $f''(0) = 1$, f has a zero of multiplicity two at $p = 0$.

Method

Define

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

If p is a zero of f of multiplicity m and $f(x) = (x - p)^m q(x)$, then

$$\mu(x) = \frac{(x - p)^m q(x)}{m(x - p)^{m-1} q(x) + (x - p)^m q'(x)} \tag{1.9}$$

$$= (x - p) \frac{q(x)}{mq(x) + (x - p)q'(x)} \tag{1.10}$$

also has a zero at p , and p is a simple zero of μ . Newton's method can then be applied to μ to give

$$g(x) = x - \frac{\mu(x)}{\mu'(x)} = x - \frac{f(x)/f'(x)}{([f'(x)]^2 - f(x)f''(x))/[f'(x)]^2} \tag{1.11}$$

$$= x - \frac{f(x)f'(x)}{[f'(x)]^2 - f(x)f''(x)} \tag{1.12}$$

Functional iteration to g will be quadratically convergent regardless of the multiplicity of the zero of f . The only drawback is the additional calculation of $f''(x)$. (py: do example)
(hw: solve $f(x) = x^3 + 4x^2 - 10 = 0$.)

1.10 Multi-variable functions

Taylor

$$F(x_{i+1}) \approx F(x_i) + \nabla F(x_i)(x_{i+1} - x_i) \tag{1.13}$$

1. Solve the linear system $J(x_i)\delta = -F(x)$ with respect to δ
2. Set $x_{i+1} = x_i + \delta$

(py: do it.) (hw: solve: $x^2 + xy = 10, y + 3xy^2 = 57$.)

1.11 Roots of Polynomials

A polynomial of degree n has the form

$$P(x) = a_n x^n + a_{n-1} x^{n-1} + \dots + a_1 x + a_0$$

where the a_i 's, called the coefficients of P , are constants and $a_n \neq 0$. The zero function $P(x) = 0$ for all values of x , is considered a polynomial but is assigned no degree.

1. ROOTS OF EQUATIONS

Fundamental Theorem of Algebra: If $P(x)$ is a polynomial of degree $n \leq 1$ with real or complex coefficients, then $P(x) = 0$ has at least one (possibly complex) root.

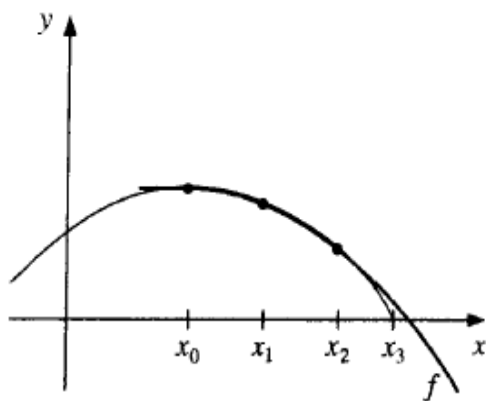
Polynomial Deflation: Remove the found root before proceeding. (here: Divide $x^2 + 2x - 24$ by the factor $x - 4$.)

When complex roots are possible, the bracketing methods cannot be used because of the obvious problem that the criterion for defining a bracket does not translate to complex guesses. Find the real and complex roots of polynomials

Theorem: If $z = a + bi$ is a complex zero of multiplicity m of the polynomial $P(x)$ with real coefficients, then $\bar{z} = a - bi$ is also a zero of multiplicity m of the polynomial $P(x)$, and $(x^2 - 2ax + a^2 + b^2)^m$ is a factor of $P(x)$.

1.12 Muller's method

Muller's method takes a similar approach that the secant method, but projects a parabola through three points



(b)

Consider the quadratic polynomial

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

that passes through $(x_0, f(x_0))$, $(x_1, f(x_1))$ and $(x_2, f(x_2))$. The constants a, b and c can be determined from the conditions

$$f(x_0) = a(x_0 - x_2)^2 + b(x_0 - x_2) + c \quad (1.14)$$

$$f(x_1) = a(x_1 - x_2)^2 + b(x_1 - x_2) + c \quad (1.15)$$

$$f(x_2) = a(0)^2 + b(0) + c = c. \quad (1.16)$$

Then,

$$c = f(x_2) \quad (1.17)$$

$$b = \frac{(x_0 - x_2)^2[f(x_1) - f(x_2)] - (x_1 - x_2)^2[f(x_0) - f(x_2)]}{(x_0 - x_2)(x_1 - x_2)(x_0 - x_1)} \quad (1.18)$$

$$c = \frac{(x_1 - x_2)^2[f(x_0) - f(x_2)] - (x_0 - x_2)^2[f(x_1) - f(x_2)]}{(x_0 - x_2)(x_1 - x_2)(x_0 - x_1)} \quad (1.19)$$

To determine x_3 (a zero of P), we apply the quadratic formula to $P(x) = 0$.

$$x_3 = x_2 + \frac{-2c}{b \pm \sqrt{b^2 - 4ac}}$$

(hw: find the roots (4) of $16x^4 - 40x^3 + 5x^2 + 20x + 6$, with 0.5, -0.5, 0, 0.5, 1.0, 1.5 and 2.5, 2, 2.25.)

Can find imaginary roots. No need to find derivatives.

Other methods: Laguerre's method, which approximates both real and complex roots and has cubic convergence, is among the best approaches.

<https://docs.scipy.org/doc/scipy/reference/optimize.html>

1. ROOTS OF EQUATIONS

Method	Type	Guesses	Convergence	Stability	Programming	Comments
Direct	Analytical	—	—	—	—	Imprecise
Graphical	Visual	—	—	—	—	
Bisection	Bracketing	2	Slow	Always	Easy	
False-position	Bracketing	2	Slow/medium	Always	Easy	
Modified FP	Bracketing	2	Medium	Always	Easy	
Fixed-point iteration	Open	1	Slow	Possibly divergent	Easy	
Newton-Raphson	Open	1	Fast	Possibly divergent	Easy	
Modified Newton-Raphson	Open	1	Fast (multiple), medium (single)	Possibly divergent	Easy	Requires evaluation of $f'(x)$
Secant	Open	2	Medium/fast	Possibly divergent	Easy	Requires evaluation of $f'(x)$ and $f''(x)$
Modified secant	Open	1	Medium/fast	Possibly divergent	Easy	Initial guesses do not have to bracket the root
Brent	Hybrid	1 or 2	Medium	Always (for 2 guesses)	Moderate	
Müller	Polynomials	2	Medium/fast	Possibly divergent	Moderate	Robust
Bairstow	Polynomials	2	Fast	Possibly divergent	Moderate	