ME 310

Numerical Methods

Finding Roots of Nonlinear Equations

These presentations are prepared by

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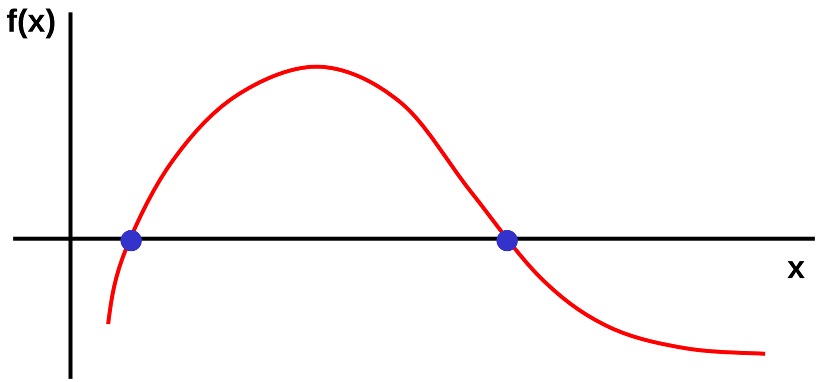
Part 2. Finding Roots of Equations

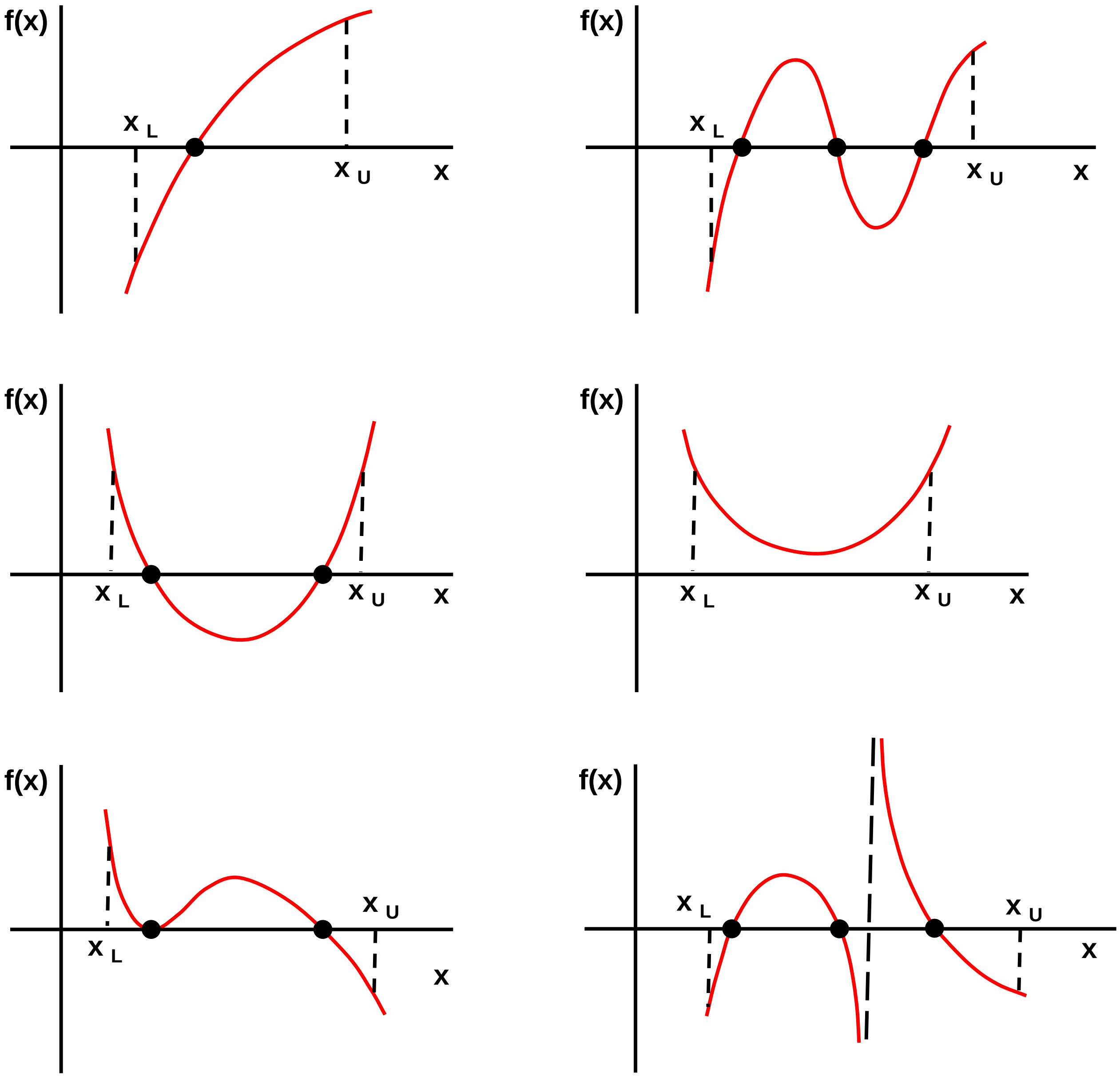


f(x) is given

$f(x_r) = 0 \quad \rightarrow \quad x_r = ?$

- Bracketing Methods (Need two initial estimates that will bracket the root. Always converge.)
  - Bisection Method
  - False-Position Method
- Open Methods (Need one or two initial estimates. May diverge.)
  - Simple One-Point Iteration
  - Newton-Raphson Method (Needs the derivative of the function.)
  - Secant Method

Ch 5. General Idea of Bracketing Methods



Rule 1: If f(x $_L$)*f(x $_U$) < 0 than there are

odd number of roots

Rule 2: If f(x $_L$)*f(x $_U$) > 0 than ther are

i) even number of roots

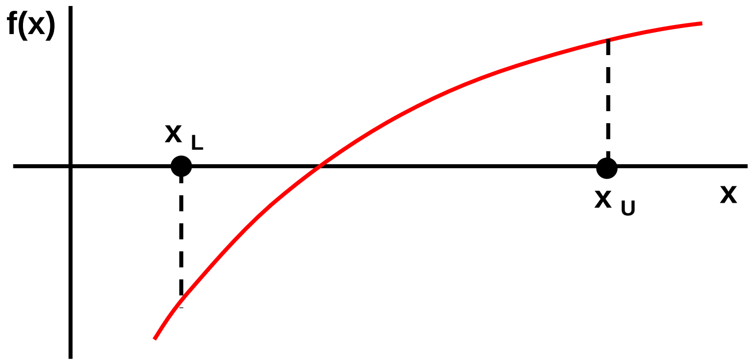
ii) no roots

Violations:

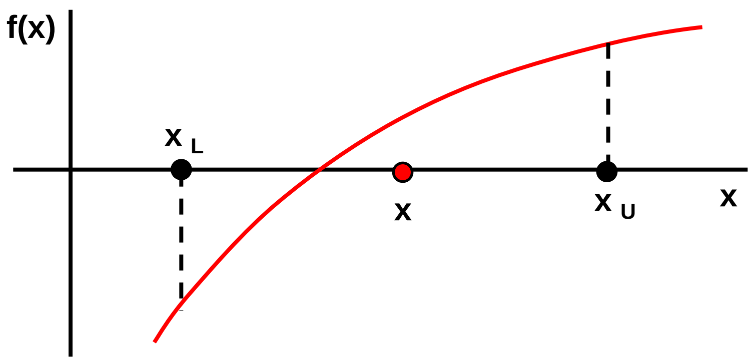
i) multiple roots

ii) discontinuities

Bisection Method

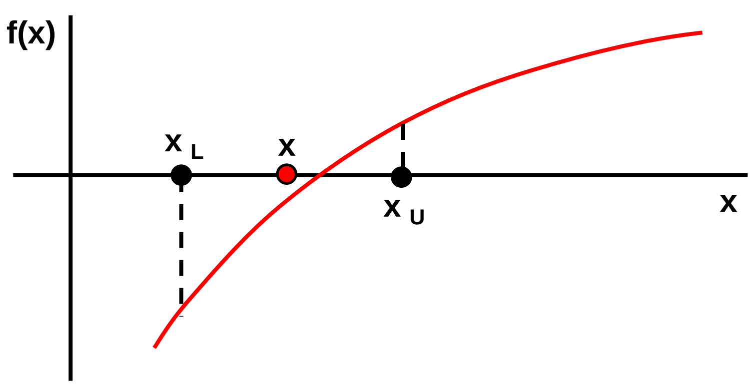


- Start with two initial guesses, x_{LOWER} and x_{UPPER} .
- They should bracket the root, i.e. $f(x_L) * f(x_U) < 0$



- Estimate the root as the midpoint of this interval. $\boxed{x= (x_L+x_U)/2}$
- Determine the interval which contains the root

if $f(x_L) * f(x) < 0$	root is between x_L and x
else	root is between x and x_U



- Estimate a new root in this new interval
- Iterate like this and compute the error after each iteration.
- Stop when the specified tolerance is reached.

Bisection Method (cont'd)

- It always converge to the true root (but be careful about the following)
- $f(x_L) * f(x_U) < 0$ is true if the interval has odd number of roots, not necessarily one root.

Example 6: Find the square root of 11.

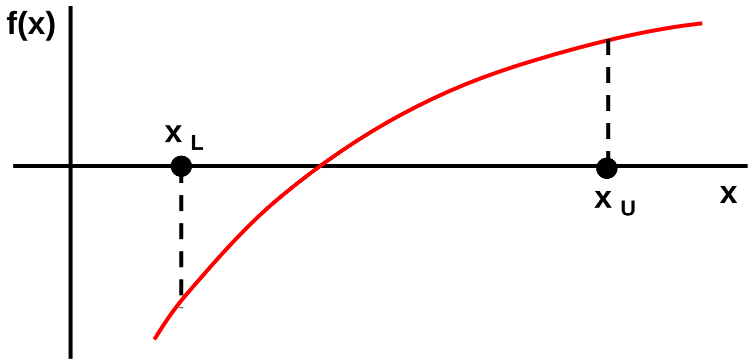
$x^2 = 11 \quad \rightarrow \quad f(x) = x^2 - 11$ (note that the exact solution is 3.31662479)

Select initial guesses: $3^2=9 < 11$, $4^2=16 > 11 \quad \rightarrow \quad x_L = 3, \; x_U = 4$

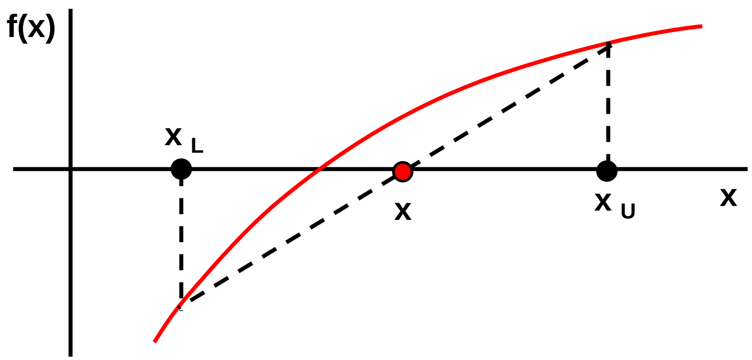
Iteration no.	x	f(x)	$\lvert\varepsilon_t\rvert$ %	$\lvert\varepsilon_a\rvert$ %
1	3.5	1.25	5.53	-----
2	3.25	-0.4375	2.01	7.69
3	3.375	0.390625	1.76	3.70
4	3.3125	-0.02734375	0.12	1.89
5	3.34375	0.180664062	0.82	0.93
6	3.328125	0.076416015	0.35	0.47

- Errors do not drop monotonically but oscillate.
- $\varepsilon_a > \varepsilon_t$ at each step, which is good. It means using ε_a is conservative.
- ε_a can also be estimated as $\varepsilon_a = (x_U - x_L)/(x_U + x_L)$. This can be used for the 1st iteration too.

False-Position Method



- Start with two initial guesses, x_{LOWER} and x_{UPPER} .
- They should bracket the root, i.e. $f(x_L) * f(x_U) < 0$



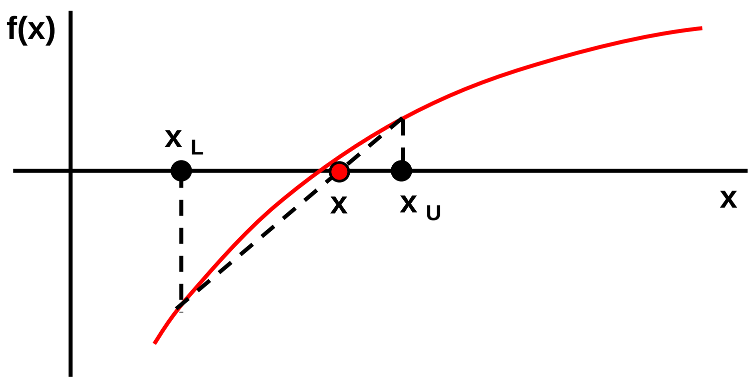
- Estimate the root using similar triangles.

$$\boxed{x = x_U - \frac{f(x_U)(x_L - x_U)}{f(x_L) - f(x_U)}}$$

- Determine the interval which contains the root

  if $f(x_L) * f(x) < 0$ root is between x_L and x

  else root is between x and x_U



- Estimate a new root in this new interval
- Iterate like this and compute the error after each iteration.
- Stop when the specified tolerance is reached.

False-Position Method (cont'd)

- It always converge to the true root.
- $f(x_L) * f(x_U) < 0$ is true if the interval has odd number of roots, not necessarily one root.
- Generally converges faster than the bisection method (See page 127 for an exception).

Example 7: Repeat the previous example (Find the square root of 11).

Iteration no.	x	f(x)	$\lvert\varepsilon_t\rvert$ %	$\lvert\varepsilon_a\rvert$ %
1	3.28571429	-0.1040816	0.932	-----
2	3.31372549	-0.0192234	0.087	0.845
3	3.31635389	-0.0017969	0.0082	0.079
4	3.31659949	-0.0001678	0.00076	0.0074
5	3.31662243	-0.0000157	0.00007	0.00069
6	3.31662457	-0.0000015	0.00001	0.00006

- Errors drop monotonically. Converges faster than the bisection method.
- $\varepsilon_a > \varepsilon_t$ at each step, which is good. It means ε_a is conservative.

About bracketing methods

- A plot of the function is always helpful.
    - to determine the number of all roots, if there are any.
    - to determine whether the roots are multiple or not.
    - to determine whether to method converges to the desired root.
    - to determine the initial guesses.

- Incremental search technique can be used to determine the initial guesses.
    - Start from one end of the region of interest.
    - Evaluate the function at specified intervals.
    - If the sign of the function changes, than there is a root in that interval.
    - Select your intervals small, otherwise you may miss some of the roots. But if they are too small, incremental search might become too costly.
    - Incremental search, just by itself, can be used as a root finding technique with very small intervals (not efficient).

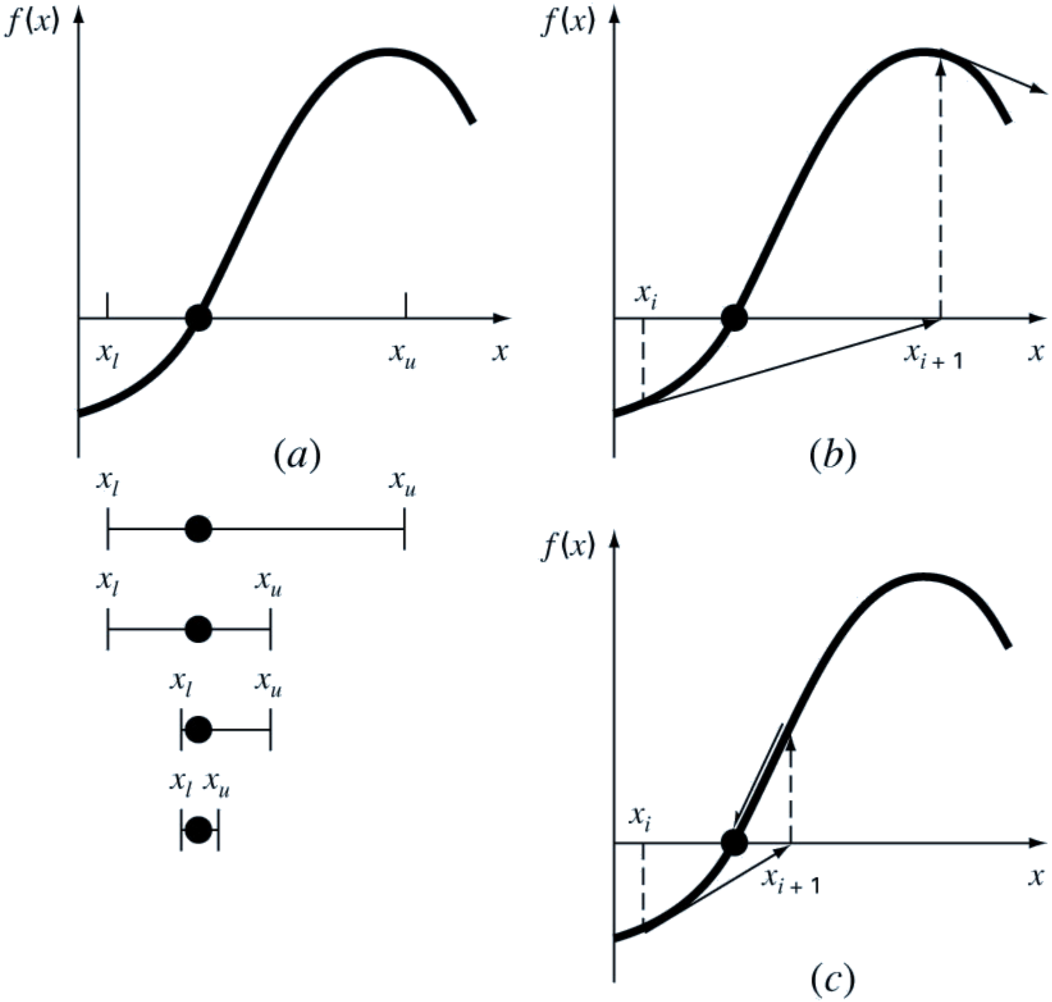
Fortran Code for Bisection Method

```
PROGRAM BISECTION    ! Calculates the root of a function

INTEGER :: iter, maxiter
REAL(8) :: xL, xU, x, fxL, fxU, fx, tol, error
READ(*,*) xL, xU, tol, maxiter

DO iter = 1, maxiter
   x = (xL + xU) / 2    ! Only this line changes for the False-Position Method
   fx = FUNC (x)        ! Call a subroutine to calculate the function.
   error = (xU - xL) / (xU + xL)*100   ! See page 121
   WRITE(*,*) iter, x, fx, error
   IF (error < tol) STOP

   fxL = FUNC (xL)
   fxU = FUNC (xU)
   IF(fxL * fx < 0) THEN
      xU = x
   ELSE
      xL = x
   ENDIF
ENDDO
END PROGRAM BISECTION
```

Exercise 5: Write a C program for the Bisection method and implement the following improvements

- Check if the initial guesses bracket the root or not.
- Read the true value if it is known and calculate ε_t in addition to ε_a.
- Check for the cases of $f(x_L)=0$ or $f(x_U)=0$

Ch 6. Open Methods



(a) Bracketing methods always converge.

(b) Open methods may diverge

(c) or converge very rapidly.

Simple One-Point Iteration

- Put the original formulation of $f(x) = 0$ into a form of $x=g(x)$.
- Many possibilities are possible
  - $\ln(x) - 3x + 5 = 0 \quad \rightarrow \quad x = [\ \ln(x) + 5\ ] / 3$ or $x = e^{3x-5}$
  - $\cos(x) = 0 \quad \rightarrow \quad x = x + \cos(x)$

- Start with an initial guess x_0
- Calculate a new estimate for the root using $x_1 = g(x_0)$
- Iterate like this. General formula is $\boxed{x_{i+1} = g(x_i)}$

- Converges if $|g'(x)|<1$ in the region of interest (Easier to see graphically in the coming slides).

Simple One-Point Iteration (cont'd)

Example 8: Repeat the previous example (Find the square root of 11). Start with $x_0 = 3$.

(a) $x^2-11 = 0 \rightarrow x = x + x^2 - 11$

i	x_i	$x_{i+1}=g(x_i)$	$\lvert\varepsilon_t\rvert$ %
0	3	1	70
1	1	-9	371
2	-9	61	1739
3	61	3771	113600
Diverges			

(b) $11-x^2 = 0 \rightarrow x = (4x+11-x^2)/4$

i	x_i	$x_{i+1}=g(x_i)$	$\lvert\varepsilon_t\rvert$ %
0	3	3.5	5.53
1	3.5	3.1875	3.89
2	3.1875	3.39746094	2.44
3	3.39746094	3.26177573	1.65
4	3.26177573	3.35198050	1.07
5	3.35198050	3.29303718	0.71
Converges			

- Selection of g(x) is important. Note that we did not use the trivial one, $x = \sqrt{11}$.
- If the method converges, convergence is linear. That is the relative error at each iteration is roughly proportional to the half of the previous error. This is easier to see for ε_t.

Exercise 6: Show that (a) violates the convergence criteria $|g'(x)|<1$.

Simple One-Point Iteration (cont'd)

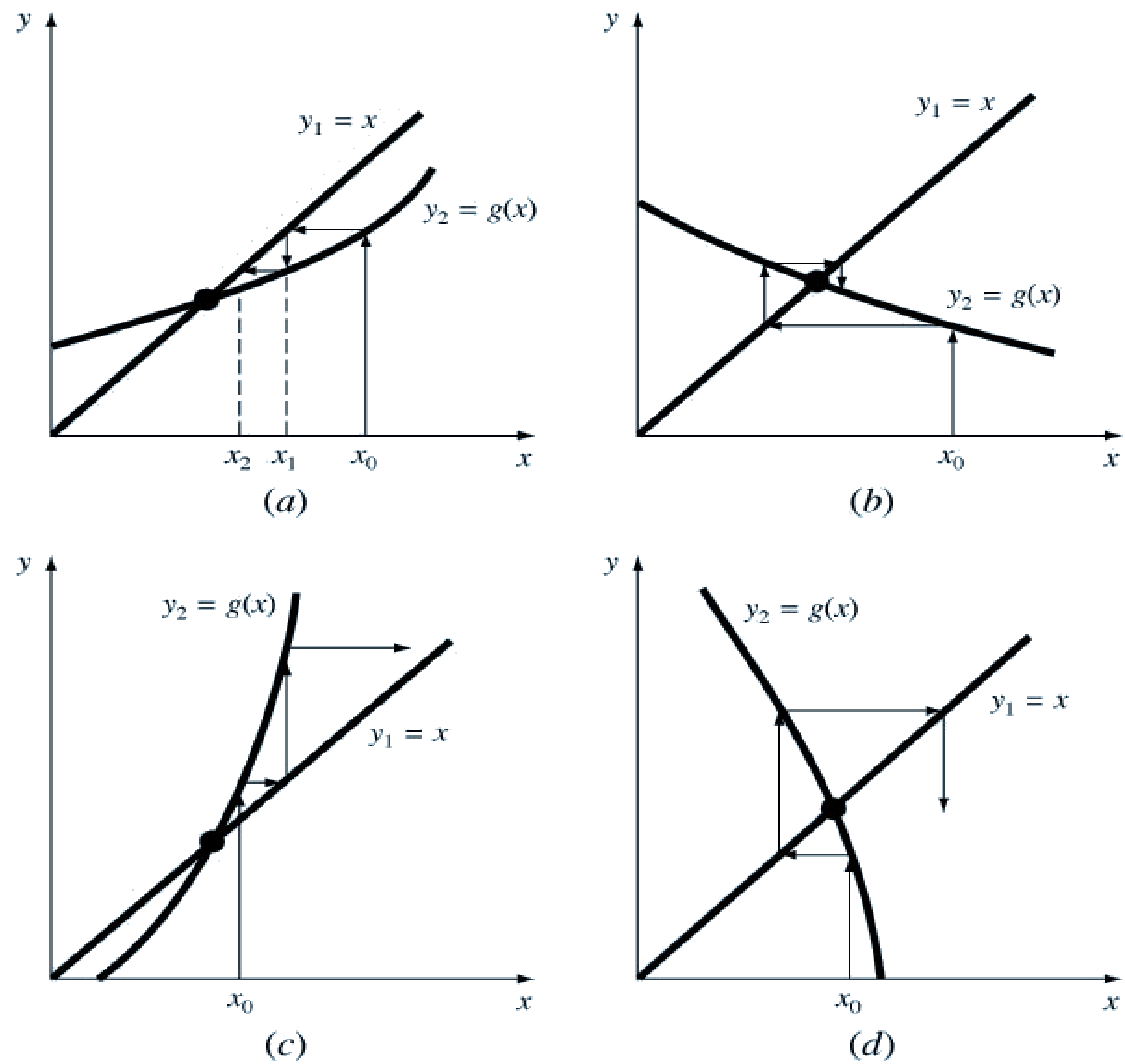
- We can use the two-curve graphical method to check convergence $|g'(x)|<1$.

(a) Monotone convergence

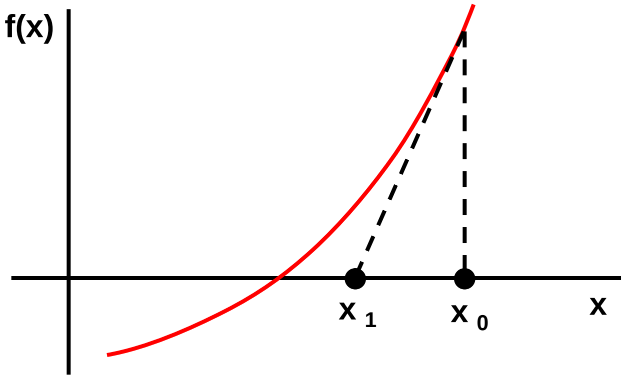
(b) Spiral convergence

(c) Monotone divergence

(d) Spiral divergence

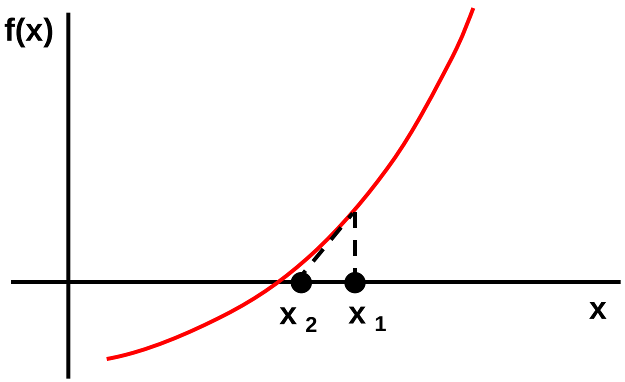


Newton-Raphson Method



- Start with an initial guess x_0 and calculate x_1 as

$$f'(x_0) = \frac{f(x_0) - 0}{x_1 - x_0} \quad \rightarrow \quad x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$



- Continue like this until you reach the specified tolerance or maximum number of iterations.

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

Newton-Raphson Method (cont'd)

Example 9: Repeat the previous example (Find the square root of 11). Start with $x_0 = 3$.

$$f(x) = x^2 - 11 = 0\ ,\ \ f'(x) = 2x \quad \rightarrow \quad x_{i+1} = x_i - (x^2 - 11)/2x$$

iter	x	f(x)	$\lvert\varepsilon_t\rvert$ %
0	3	-2	9.55
1	3.33333333	0.1111111	0.50
2	3.31666667	0.0002778	0.00126
3	3.31662479	0.0000000	0.00000

Selection of the initial guess affects the convergence a lot.

Exercise 7: NR method is quite sensitive to the starting point. Try to find the first positive root of sin(x) (which is 1.570796) starting with a) $x_0 = 1.5$, b) $x_0 = 1.7$, c) $x_0 = 1.8$, d) $x_0 = 1.9$ (They all converge to different roots).

Derivation of NR Method from Taylor Series

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

Use first order approximation $\rightarrow$ $f(x_{i+1}) \approx f(x_i) + f'(x_i)(x_{i+1} - x_i)$

To find the root, $f(x_{i+1})$ should be zero $\rightarrow$ $0 \approx f(x_i) + f'(x_i)(x_{i+1} - x_i)$

Solve for x_{i+1} $\rightarrow$ $x_{i+1} = x_i - \dfrac{f(x_i)}{f'(x_i)}$

Error Analysis

If we use the complete Taylor Series the result would be exact.

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

x_e is the exact root

Subtract this from the 3rd equation $\rightarrow$ $0 = f'(x_i)(x_e - x_{i+1}) + \dfrac{f''(\xi)}{2}(x_e - x_i)^2$

Note that $E_{t,i} = (x_e - x_i)$ and $E_{t,i+1} = (x_e - x_{i+1})$ $\rightarrow$ $0 = f'(x_i)E_{t,i+1} + \dfrac{f''(\xi)}{2}E_{t,i}^2$

For convergence both x_i and ξ should approach to x_e $\rightarrow$ $E_{t,i+1} \approx \dfrac{f''(x_e)}{2f'(x_e)}E_{t,i}^2$

This is quadratic convergence. That is the error at each iteration is roughly proportional to the square of the previous error. (See page 141 for a nice example).

Exercise 8: We showed that the NR can be derived from a 1^{st} order Taylor series expansion. Derive a new method using 2^{nd} order Taylor series expansion. Compare the convergence of this method with NR. Comment on the practicality of this new method.

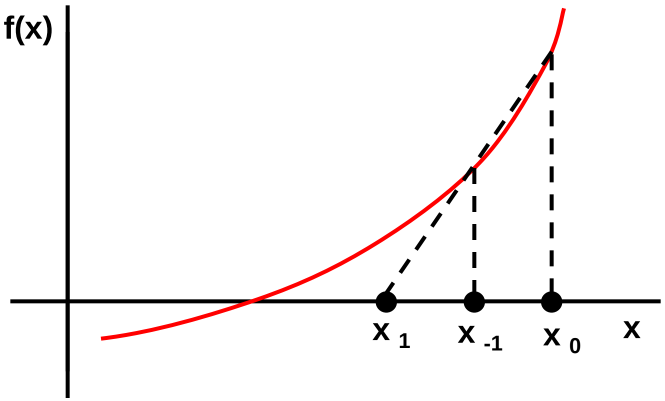
Exercise 9: NR method can be seen as Simple One-Point Iteration method with $g(x) = x_i - f(x_i) / f'(x_i)$. Using the convergence criteria of the Simple One-Point Iteration Method, derive a convergence criteria for the NR Method.

Difficulties with the NR Method (page 144)

- Need to know the derivative of the function.
- May diverge around inflection points.
- May give oscillations around local minimums or maximums.
- Zero or near zero slope is a problem, because f' is at the denominator.
- Convergence may be slow if the initial guess is poor.

Exercise 9.1 : Use the NR method to locate one of the roots of $f(x) = x(x-5)(x-6)+3$ starting with $x_0 = 3.5$ (NR will oscillate around the local minimum).

Secant Method

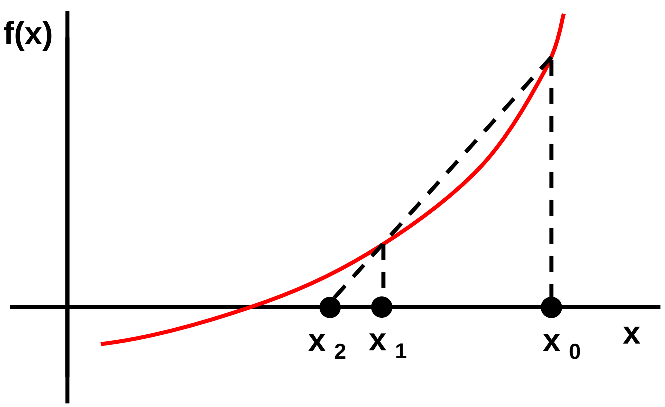


- Start with two initial guess x_{-1} and x_0.

$$f'(x_0) \approx \frac{f(x_{-1}) - f(x_0)}{x_{-1} - x_0}$$

Use this in the equation of NR method.

$$x_1 = x_0 - \frac{f(x_0)(x_{-1} - x_0)}{f(x_{-1}) - f(x_0)}$$



- Continue like this until you reach the specified tolerance or maximum number of iterations.

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

Secant Method (cont'd)

Example 10: Repeat the same example (Find the square root of 11).

Start with $x_{-1} = 2$, $x_0 = 3$

$f(x) = x^2 - 11 = 0$

iter	x	f(x)	$\lvert\varepsilon_t\rvert$ %
-1	2	-7	-311
0	3	-2	-160
1	3.4	0.56	2.51
2	3.3125	-0.0273438	0.12
3	3.31657356	-0.0003398	0.0015
4	3.31662482	0.0000002	0.0000

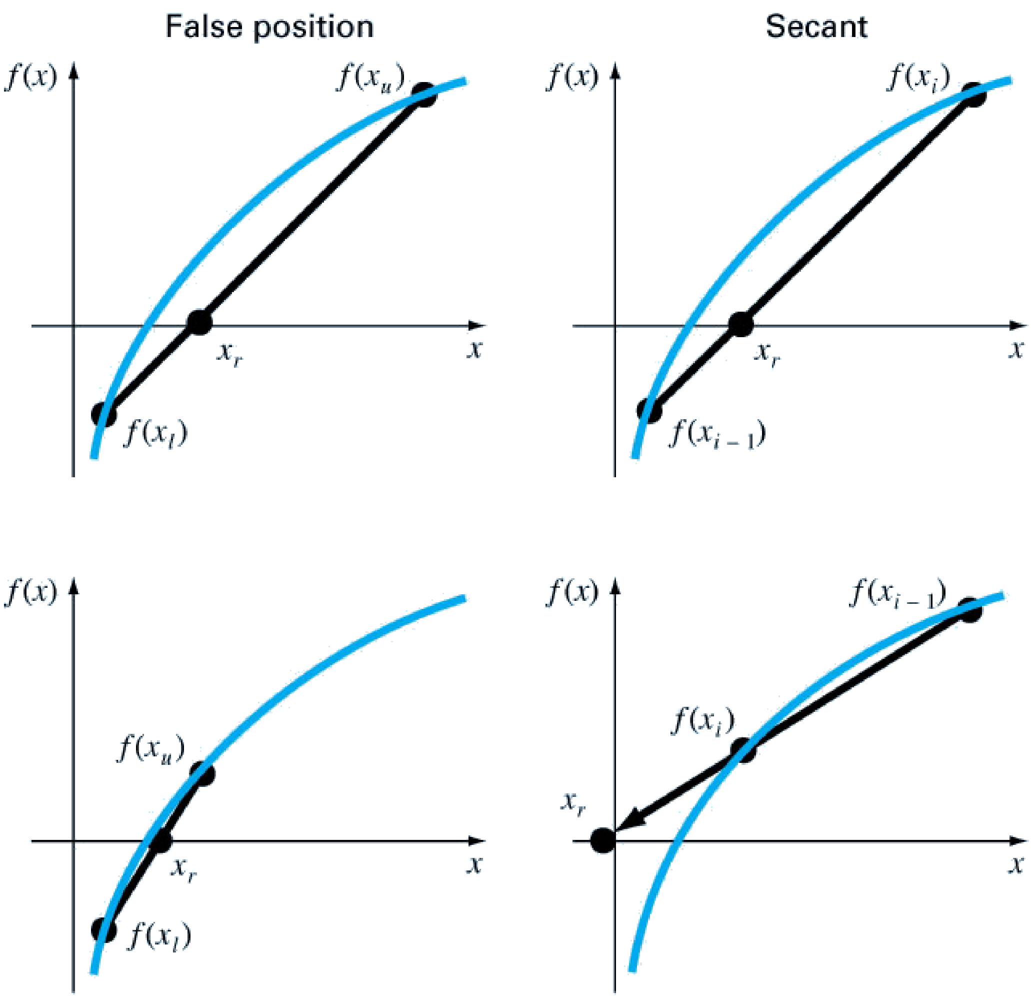
Selection of the initial guess affects the convergence a lot.

Exercise 10: There is no guarantee for the secant method to converge. Try to calculate the root of ln(x) starting with (a) $x_{-1} = 0.5$ and $x_0 = 4$, (b) $x_{-1} = 0.5$ and $x_0 = 5$. Part (a) converges, but not part (b)

Secant vs. False Position

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

False-Position: $$x = x_U - \frac{f(x_U)(x_L - x_U)}{f(x_L) - f(x_U)}$$



First iterations of both methods are the same.

Second iterations are different in terms of how the previous estimates are replaced with the newly calculated root.

- False-position Method drops one of previous estimates so that the reamining ones bracket the root.

- Secant Method always drops the oldest estimate.

Special Treatment of Multiple Roots

- At even multiple roots, bracketing methods can not be used at all.

- Open methods still work but
  - $f'(x)$ also goes to zero at a multiple root. Possibility of division by zero for Secant and NR. $f(x)$ will reach zero faster than $f'(x)$, therefore use a zero-check for $f(x)$ and stop properly.
  - they converge slowly (linear instead of quadratic convergence).

- Some modifications can be made for speed up.

  i) If you know the multiplicity of the root NR can be modified as

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

m=2 for a double root, m=3 for a triple root, etc.

  ii) Another alternative is to define a new function $u(x)=f(x)/f'(x)$ and use it in the formulation of NR Method

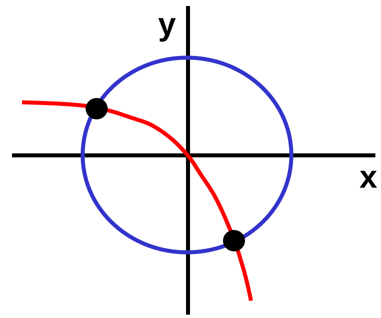
$$\mathbf{x_{i+1} = x_i - \frac{u(x_i)}{u'(x_i)} = \frac{f(x_i)f'(x_i)}{[f'(x_i)]^2 - f(x_i)f''(x_i)}}$$

You need to know $f''(x)$

(Similar modifications can be made for the Secant Method. See the book for details.)

Solving System of Nonlinear Equations

Using Simple One-Point Iteration Method



Solve the following system of equations

$$x^2 + y^2 = 4$$
$$e^x + y = 1$$

Put the functions into the form $x=g_1(x,y)$, $y=g_2(x,y)$

$$x = g_1(y) = \ln(1 - y)$$
$$y = g_2(x) = -\sqrt{4 - x^2}$$

Select a starting values for x and y, such as $x_0=0.0$ and $y_0=0.0$. They don't need to satisfy the equations. Use these values in g functions to calculate new values.

$x_1= g_1(y_0) = 0$ $\quad$ $y_1= g_2(x_1) = -2$

$x_2= g_1(y_1) = 1.098612289$ $\quad$ $y_2= g_2(x_2) = -1.67124236$

$x_3= g_1(y_2) = 0.982543669$ $\quad$ $y_3= g_2(x_3) = -1.74201261$

$x_4= g_1(y_3) = 1.00869218$ $\quad$ $y_4= g_2(x_4) = -1.72700321$

The solution is converging to the exact solution of $x=1.004169$, $y=-1.729637$

Exercise 11: Solve the same system but rearrange the equations as $x=\ln(1-y)$ $\quad$ $y = (4-x^2)/y$ and start from $x_0=1$ $y_0=-1.7$. Remember that this method may diverge.

Solving System of Nonlinear Equations

Using Newton-Raphson Method

Consider the following general form of a two equation system

$$u(x, y) = 0$$
$$v(x, y) = 0$$

Write 1st order TSE for these equations

$$u_{i+1} = u_i + \frac{\partial u_i}{\partial x}(x_{i+1} - x_i) + \frac{\partial u_i}{\partial y}(y_{i+1} - y_i)$$
$$v_{i+1} = v_i + \frac{\partial v_i}{\partial x}(x_{i+1} - x_i) + \frac{\partial v_i}{\partial y}(y_{i+1} - y_i)$$

To find the solution set $u_{i+1} = 0$ and $v_{i+1} = 0$. Rearrange

$$\frac{\partial u_i}{\partial x}x_{i+1} + \frac{\partial u_i}{\partial y}y_{i+1} = -u_i + \frac{\partial u_i}{\partial x}x_i + \frac{\partial u_i}{\partial y}y_i$$
$$\frac{\partial v_i}{\partial x}x_{i+1} + \frac{\partial v_i}{\partial y}y_{i+1} = -v_i + \frac{\partial v_i}{\partial x}x_i + \frac{\partial v_i}{\partial y}y_i$$

$$\begin{bmatrix} \frac{\partial u_i}{\partial x} & \frac{\partial u_i}{\partial y} \\ \frac{\partial v_i}{\partial x} & \frac{\partial v_i}{\partial y} \end{bmatrix} \begin{Bmatrix} x_{i+1} \\ y_{i+1} \end{Bmatrix} = \begin{Bmatrix} -u_i + \frac{\partial u_i}{\partial x}x_i + \frac{\partial u_i}{\partial y}y_i \\ -v_i + \frac{\partial v_i}{\partial x}x_i + \frac{\partial v_i}{\partial y}y_i \end{Bmatrix}$$

The first matrix is called the Jacobian matrix.

Solve for x_{i+1}, y_{i+1} and iterate.

Can be generalized for n simultaneous equations

Solving System of Eqns Using NR Method (cont'd)

Solve for x_{i+1} and y_{i+1} using Cramer's rule (ME 210)

$$x_{i+1} = x_i - \frac{u_i \frac{\partial v_i}{\partial y} - v_i \frac{\partial u_i}{\partial y}}{\frac{\partial u_i}{\partial x}\frac{\partial v_i}{\partial y} - \frac{\partial u_i}{\partial y}\frac{\partial v_i}{\partial x}} \quad , \quad y_{i+1} = y_i - \frac{v_i \frac{\partial u_i}{\partial x} - u_i \frac{\partial v_i}{\partial x}}{\frac{\partial u_i}{\partial x}\frac{\partial v_i}{\partial y} - \frac{\partial u_i}{\partial y}\frac{\partial v_i}{\partial x}}$$

The denominator is the determinant of the Jacobian matrix |J|.

Example 11: Solve the same system of equations

$$u = x^2 + y^2 - 4 = 0$$
$$v = e^x + y - 1 = 0$$

stating with x_0=1, y_0=1

$$\frac{\partial u}{\partial x} = 2x \;,\; \frac{\partial u}{\partial y} = 2y \;,\; \frac{\partial v}{\partial x} = e^x \;,\; \frac{\partial v}{\partial y} = 1 \;\rightarrow\; |J| = 2x - 2ye^x$$

$$x_{i+1} = x_i - \frac{u_i - 2y_i v_i}{|J|} \;,\; y_{i+1} = y_i - \frac{2xv_i - e^{x_i} u_i}{|J|}$$

i=0,	x_0=1	y_0=1	u_0=-2	v_0=2.718282	$\|J_0\|$=-3.436564
i=1,	x_1=-1.163953	y_1=3.335387	u_1=8.479595	v_1=2.647636	$\|J_1\|$=-4.410851
i=2,	x_2=-3.245681	y_2=1.337769	u_2=8.324069	v_2=0.376711	$\|J_2\|$=-6.595552
i=3,	x_3=-2.136423	y_3=0.959110	u_3=1.484197	v_3=0.077187	$\|J_3\|$=-4.499343

Looks like it is converging to the root in the 2nd quadrant $x \approx -1.8$, $y \approx 0.8$.

Exercise 12: Can you start with x_0=0 and y_0=0 ?

Exercise 13: Try to find starting points that will converge to the solution in the 4th quadrant.