

Numerical Methods for Engineers

SEVENTH EDITION

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Chapter 6

Roots of Equations Part 2 Open Methods

Simple Fixed-point Iteration

- Rearrange the function so that x is on the left side of the equation:

$$f(x) = 0 \Rightarrow g(x) = x$$

$$x_k = g(x_{k-1}) \quad x_0 \text{ given, } k = 1, 2, \dots$$

- Bracketing methods are “convergent”.
- Fixed-point methods may sometime “diverge”, depending on the stating point (initial guess) and how the function behaves.

Example:

$$f(x) = x^2 - x - 2 \quad x > 0$$

$$g(x) = x^2 - 2$$

or

$$g(x) = \sqrt{x + 2}$$

or

$$g(x) = 1 + \frac{2}{x}$$

⋮

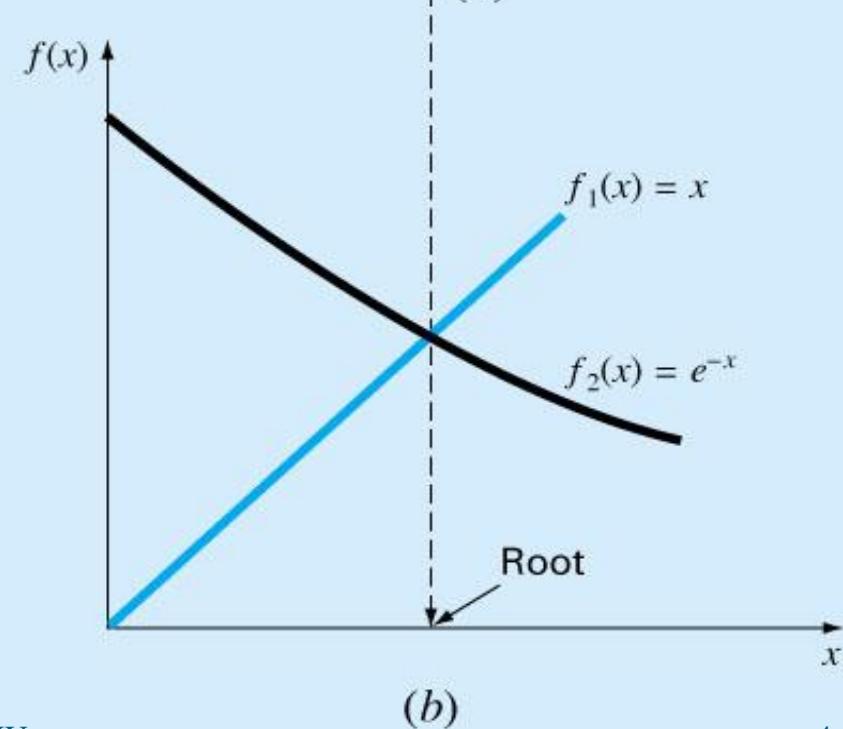
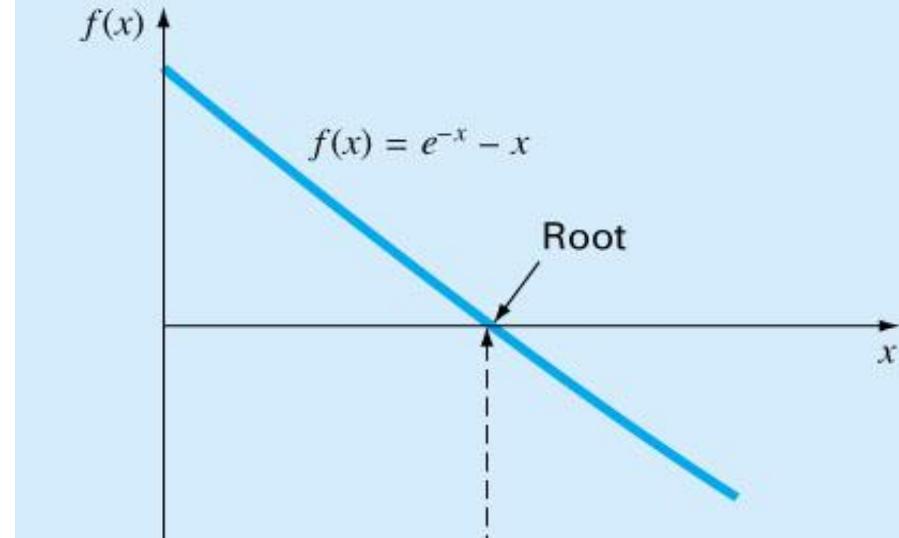
Convergence

- $x=g(x)$ can be expressed as a pair of equations:

$$y_1=x$$

$$y_2=g(x) \text{ (component equations)}$$

- Plot them separately.



Conclusion

- Fixed-point iteration converges if

$$|g'(x)| < 1 \quad (\text{slope of the line } f(x) = x)$$

- When the method converges, the error is roughly proportional to or less than the error of the previous step, therefore it is called “linearly convergent.”

Newton's Method-Overview

- Open search method
- A good initial estimate of the solution is required
- The objective function must be twice differentiable
- Unlike Golden Section Search method
 - Lower and upper search boundaries are not required (open vs. bracketing)
 - May not converge to the optimal solution
- Most widely used method.
- Based on Taylor series expansion

$$f(x_{i+1}) = f(x_i) + f'(x_i)\Delta x + f''(x_i) \frac{\Delta x^2}{2!} + O\Delta x^3$$

The root is the value of x_{i+1} when $f(x_{i+1}) = 0$

Rearranging,

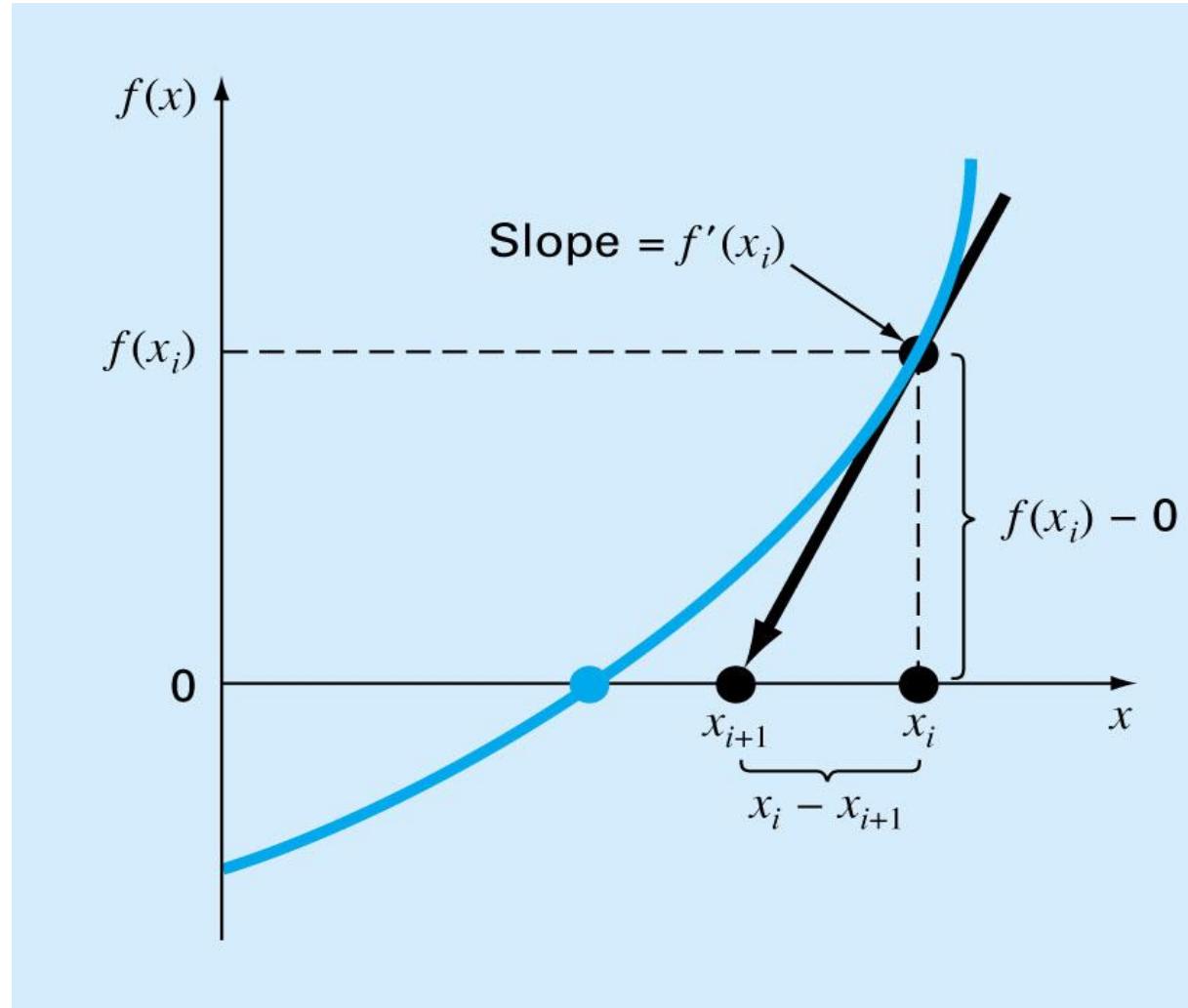
$$0 = f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

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

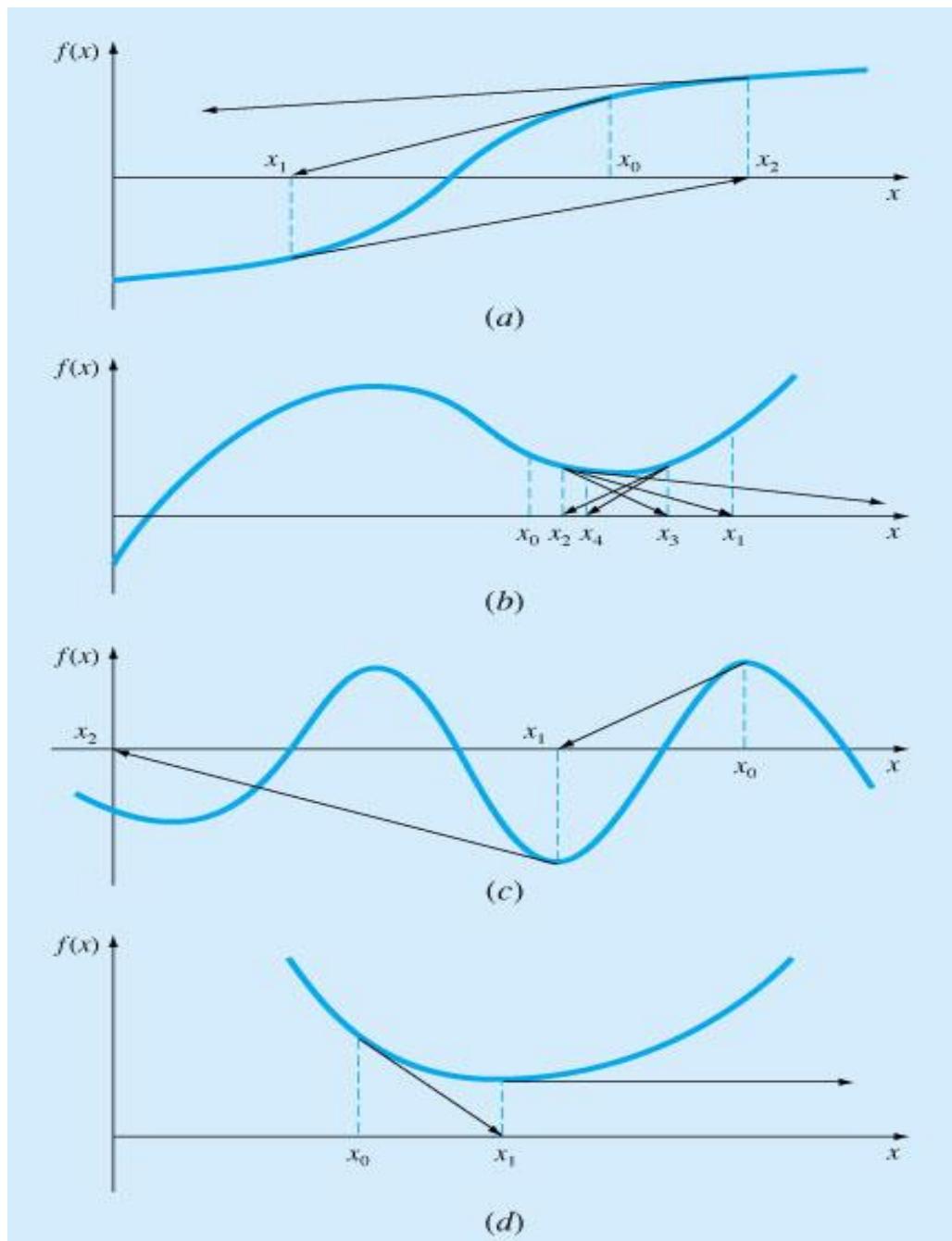
Solve for

Newton-Raphson formula

A convenient method for functions whose derivatives can be evaluated analytically. It may not be convenient for functions whose derivatives cannot be evaluated analytically.



How it diverge



Newton's Method-How it works

- The derivative of the function $f(x)$, $f'(x)=0$ at the function's maximum and minimum.
- The minima and the maxima can be found by applying the Newton-Raphson method to the derivative, essentially obtaining

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

Newton's Method-Algorithm

Initialization: Determine a reasonably good estimate for the maxima or the minima of the function $f(x)$.

Step 1. Determine $f'(x)$ and $f''(x)$.

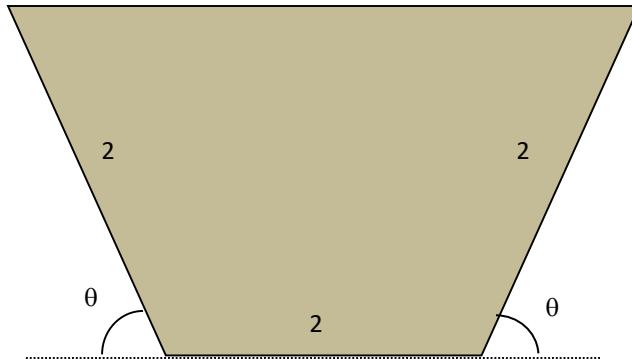
Step 2. Substitute x_i (initial estimate x_0 for the first iteration) $f'(x)$ and $f''(x)$ into

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

to determine x_{i+1} and the function value in iteration i .

Step 3. If the value of the first derivative of the function is zero then you have reached the optimum (maxima or minima). Otherwise, repeat Step 2 with the new value of

Example



The cross-sectional area A of a gutter with equal base and edge length of 2 is given by

$$A = 4 \sin \theta (1 + \cos \theta)$$

Find the angle θ which maximizes the cross-sectional area of the gutter.

Solution

The function to be maximized is $f(\theta) = 4 \sin \theta (1 + \cos \theta)$

$$f'(\theta) = 4(\cos \theta + \cos^2 \theta - \sin^2 \theta)$$

$$f''(\theta) = -4 \sin \theta (1 + 4 \cos \theta)$$

Iteration 1: Use $\theta_0 = \pi/4$ as the initial estimate of the solution

$$\theta_1 = \frac{\pi}{4} - \frac{4(\cos \frac{\pi}{4} + \cos^2 \frac{\pi}{4} - \sin^2 \frac{\pi}{4})}{-4 \sin \frac{\pi}{4} (1 + 4 \cos \frac{\pi}{4})} = 1.0466$$

$$f(1.0466) = 5.196151$$

Solution Cont.

Iteration 2:

$$\theta_2 = 1.0466 - \frac{4(\cos 1.0466 + \cos^2 1.0466 - \sin^2 1.0466)}{-4 \sin 1.0466(1 + 4 \cos 1.0466)} = 1.0472$$

Summary of iterations

Iteration	θ	$f'(\theta)$	$f''(\theta)$	$\theta estimate$	$f(\theta)$
1	0.7854	2.8284	-10.8284	1.0466	5.1962
2	1.0466	0.0062	-10.3959	1.0472	5.1962
3	1.0472	1.06E-06	-10.3923	1.0472	5.1962
4	1.0472	3.06E-14	-10.3923	1.0472	5.1962
5	1.0472	1.3322E-15	-10.3923	1.0472	5.1962

Remember that the actual solution to the problem is at 60 degrees or 1.0472 radians.

The Newton-Raphson method suffers from four basic limitations:

- (1) Some functions are not easy to differentiate.
- (2) If the root is zero then the derivative slowly approaches zero.
- (3) If the assumed root (initial guess) is taken in an interval containing a local maximum point then the method will oscillate.
- (4) An interval contains an inflection point might cause problems, especially if the initial guess is not close to the exact root.

The Secant Method

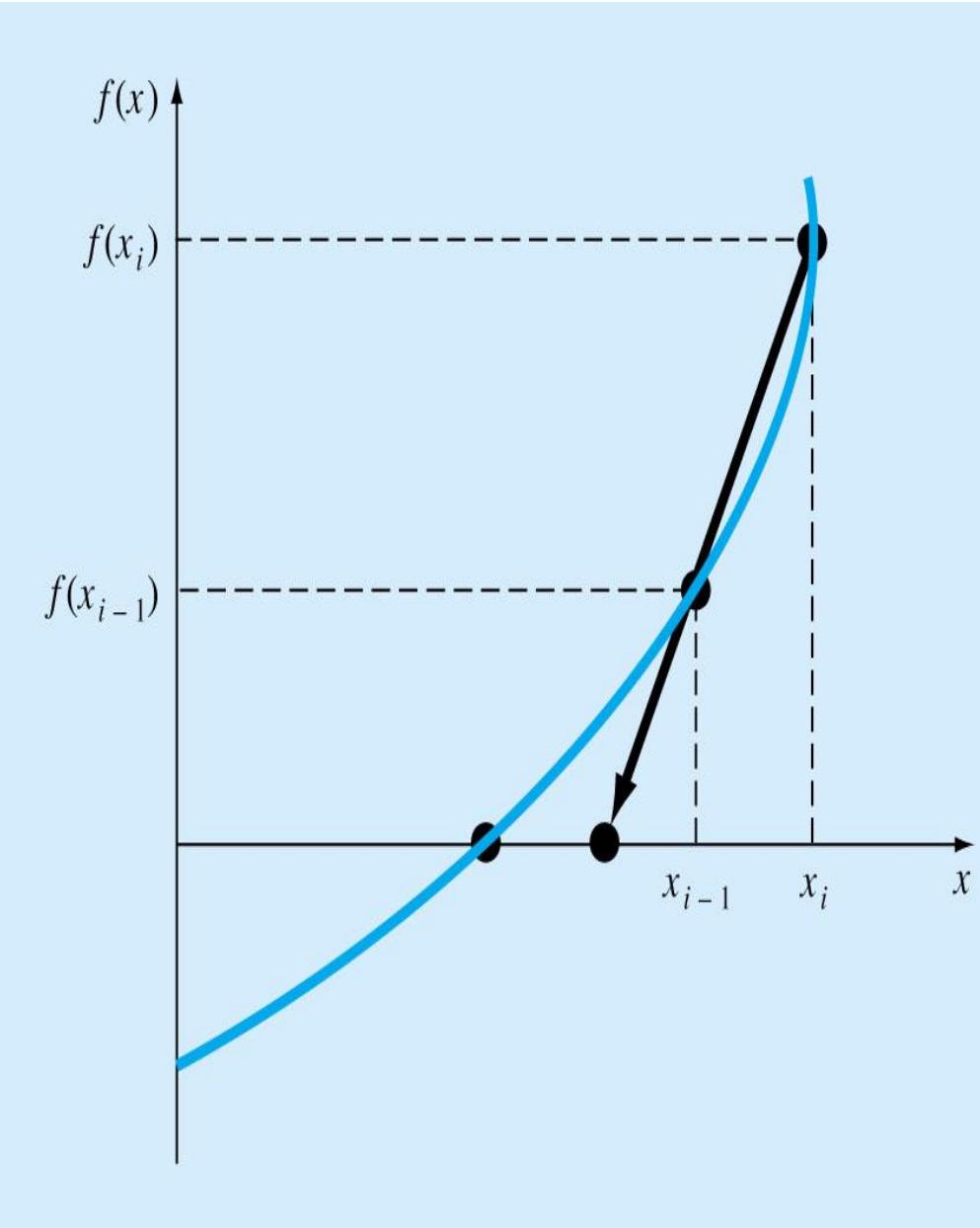
- A slight variation of Newton's method for functions whose derivatives are difficult to evaluate. For these cases the derivative can be approximated by a backward finite divided difference.

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

$$x_{i+1} = x_i - f(x_i) \frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})} \quad i = 1, 2, 3, \dots$$

Requires two initial estimates of x , e.g., x_0, x_1 . However, because $f(x)$ is not required to change signs between estimates, it is not classified as a “bracketing” method.

The secant method has the same properties as Newton’s method. Convergence is not guaranteed for all $x_0, f(x)$.



Multidimensional Newton Method

Problem : Find x^* such that $F(x^*) = 0$

$$F(\mathbf{x}) = F(\mathbf{x}^*) + J(\mathbf{x}^*)(\mathbf{x} - \mathbf{x}^*)$$

Taylor Series

$$J(\mathbf{x}) = \begin{bmatrix} \frac{\partial F_1(\mathbf{x})}{\partial x_1} & \dots & \frac{\partial F_1(\mathbf{x})}{\partial x_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_N(\mathbf{x})}{\partial x_1} & \dots & \frac{\partial F_N(\mathbf{x})}{\partial x_N} \end{bmatrix}$$

Jacobian Matrix

$$\Rightarrow \mathbf{x}^{k+1} = \mathbf{x}^k - J(\mathbf{x}^k)^{-1} F(\mathbf{x}^k)$$

Iteration function

Multidimensional Newton Method

Computational Aspects

$$\text{Iteration : } x^{k+1} = x^k - J(x^k)^{-1} F(x^k)$$

Do not compute $J(x^k)^{-1}$ (it is not sparse).

Instead solve : $J(x^k)(x^{k+1} - x^k) = -F(x^k)$

Each iteration requires:

1. Evaluation of $F(x^k)$
2. Computation of $J(x^k)$
3. Solution of a linear system of algebraic equations whose coefficient matrix is $J(x^k)$ and whose RHS is $-F(x^k)$

Multidimensional Newton Method

Algorithm

x^0 = Initial Guess, $k = 0$

Repeat { Compute $F(x^k)$, $J_F(x^k)$

Solve $J_F(x^k)(x^{k+1} - x^k) = -F(x^k)$ for x^{k+1}
 $k = k + 1$

} Until $\|x^{k+1} - x^k\|$, $\|f(x^{k+1})\|$ small enough

Example, Use the multiple-equation Newton-Raphson method to determine roots of

$$x^2 + xy = 10$$

$$y + 3xy^2 = 57$$

These equations are two simultaneous nonlinear equations with two unknowns, x and y . They can be expressed in the form of Eq. (6.17) as

$$F_1(x, y) = x^2 + xy - 10 = 0$$

$$F_2(x, y) = y + 3xy^2 - 57 = 0$$

Thus, the Jacobian matrix can be expressed as

$$J(x, y) = \begin{bmatrix} \frac{\partial F_1(x, y)}{\partial x} & \frac{\partial F_1(x, y)}{\partial y} \\ \frac{\partial F_2(x, y)}{\partial x} & \frac{\partial F_2(x, y)}{\partial y} \end{bmatrix} = \begin{bmatrix} 2x + y & x \\ 3y^2 & 1 + 6xy \end{bmatrix}$$

The inverse of the Jacobian can be expressed as

$$J^{-1}(x, y) = \frac{1}{\left[(2x + y)(1 + 6xy) - 3xy^2 \right]} \begin{bmatrix} 1 + 6xy & -x \\ -3y^2 & 2x + y \end{bmatrix}$$

Applying the iteration Equation

$$\begin{bmatrix} x^{k+1} \\ y^{k+1} \end{bmatrix} = \begin{bmatrix} x^k \\ y^k \end{bmatrix} - J^{-1}(x, y) \begin{bmatrix} F_1(x^k, y^k) \\ F_2(x^k, y^k) \end{bmatrix}$$

Note that a correct pair of roots is $x = 2$ and $y = 3$. **Initiate the computation with guesses of $x = 1.5$ and $y = 3.5$ (optional)**

$$\text{for } k = 0 \Rightarrow \begin{bmatrix} x^1 \\ y^1 \end{bmatrix} = \begin{bmatrix} 1.5 \\ 3.5 \end{bmatrix} - J^{-1}(1.5, 3.5) \begin{bmatrix} F_1(1.5, 3.5) \\ F_2(1.5, 3.5) \end{bmatrix} = \begin{bmatrix} 2.054901961 \\ 2.999620775 \end{bmatrix}$$

$$\begin{aligned} \text{for } k = 1 \Rightarrow \begin{bmatrix} x^2 \\ y^2 \end{bmatrix} &= \begin{bmatrix} 2.054901961 \\ 2.999620775 \end{bmatrix} - J^{-1}(2.054901961, 2.999620775) \begin{bmatrix} F_1(2.054901961, 2.999620775) \\ F_2(2.054901961, 2.999620775) \end{bmatrix} \\ &= \begin{bmatrix} 2.000533471 \\ 2.999999894 \end{bmatrix} \end{aligned}$$

$$\begin{aligned} \text{for } k = 2 \Rightarrow \begin{bmatrix} x^3 \\ y^3 \end{bmatrix} &= \begin{bmatrix} 2.000533471 \\ 2.999999894 \end{bmatrix} - J^{-1}(2.000533471, 2.999999894) \begin{bmatrix} F_1(2.000533471, 2.999999894) \\ F_2(2.000533471, 2.999999894) \end{bmatrix} \\ &= \begin{bmatrix} 2.000000051 \\ 3.000000000 \end{bmatrix} \end{aligned}$$

Maple Code of the previous example

```
restart;
with(linalg):
NI:=4;
F1:=x^2+x*y-10;
F2:=y+3*x*y^2-57;
JJ:=matrix(2,2,[[diff(F1,x),diff(F1,y)],[diff(F2,x),diff(F2,y)]]);
JJinv:=inverse(JJ);
F:=matrix(2,1,[[F1],[F2]]);
x0:=1.5;
y0:=3;
for i from 1 by 1 while i <=NI do
print(i);
X0:=matrix(2,1,[[x0],[y0]]);
SS:=multiply(JJinv, F);
X:=matadd(X0,-1*SS);
x0:=subs(x=x0,y=y0,X[1,1]);
y0:=subs(x=x0,y=y0,X[2,1]);
end do;
```

Homework: Edition 6

- **5.4; 5.15; 5.16**
- **6.7; 6.9; 6.16**
- **The problem in the next slide**

C= SN/100000, where SN is your student number

Given the sine-polynomial;

$$P(x) = -(C/25)x^2 \sin^5 x + (-x^5 + 2 - 4x^2) \sin^3 x + \\ (2x^5 - 2x - 2x^4) \sin^2 x + (3x + 2x^4 - 4 - x^2 - 4x^5) \sin x + \\ 2 + 8x^5 - 4x^4 - 7x^3 - x + (C/27)x^2$$

Knowing that this function has three roots in the interval [-1.5, 2.5], to be sure plot the given function over that interval. Find the roots of the above polynomial correct to 100 SFs **Using Maple** :

- i.** Find the roots using the bisection method (how many iterations needed).
- ii.** Find them using the Newton Raphson method (how many iterations needed).
- iii.** Find them using the secant method (how many iterations needed).
- iv.** Find them using the Newton's second formula (how many iterations needed) which is given as:

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

- v.** Compare between the results and the methods of parts **(i to iv)**. 26