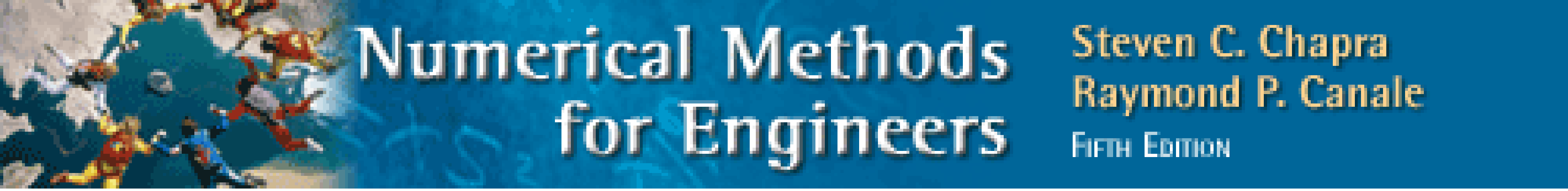


Chapter6

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:

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

$$x_k = g(x_{k-1}) \qquad x_o \text{ given, k} = 1, 2, \ldots$$

•Bracketing methods are "convergent".

•Fixed-point methods may sometime "diverge", depending on the stating point (initial guess) and how the function behaves.

Example:

$$f(x) = x^2 - x - 2 \qquad x \succ 0$$

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

or

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

or

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

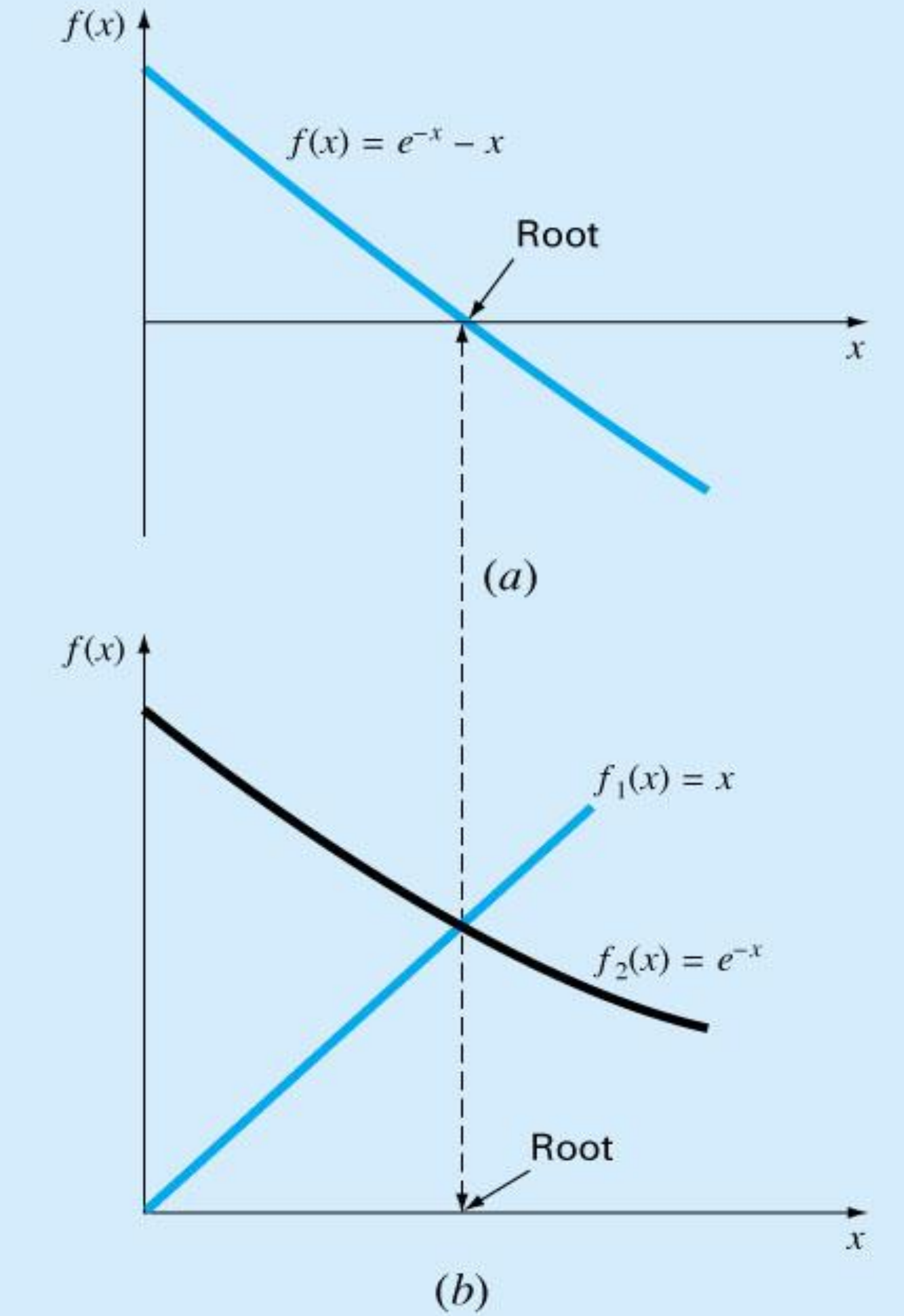
$\vdots$

Convergence

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

  $y_1=x$

  $y_2=g(x)$ (component equations)
- Plot them separately.



Conclusion

- Fixed-point iteration converges if

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

•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,

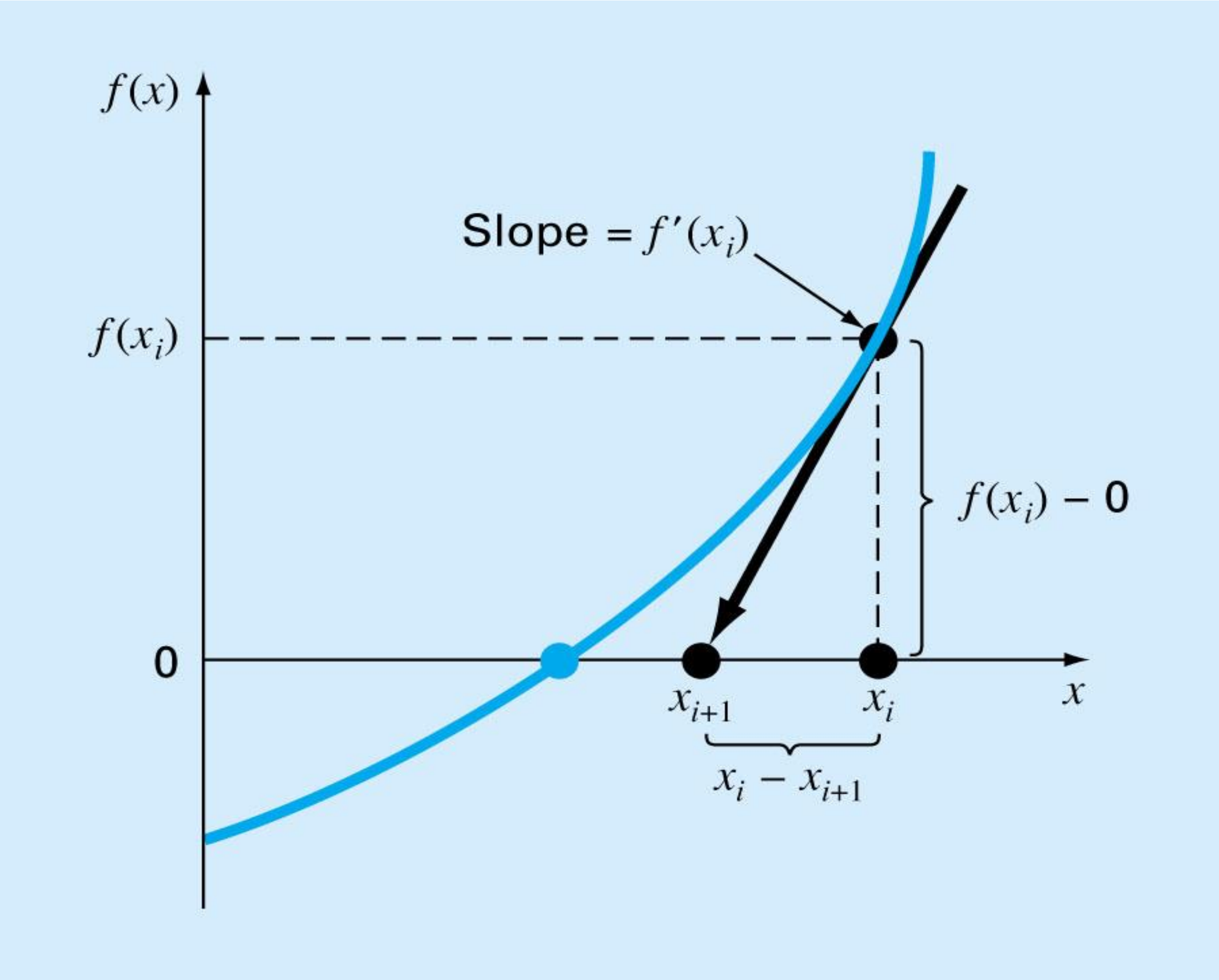
$$0 = f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

Solve for

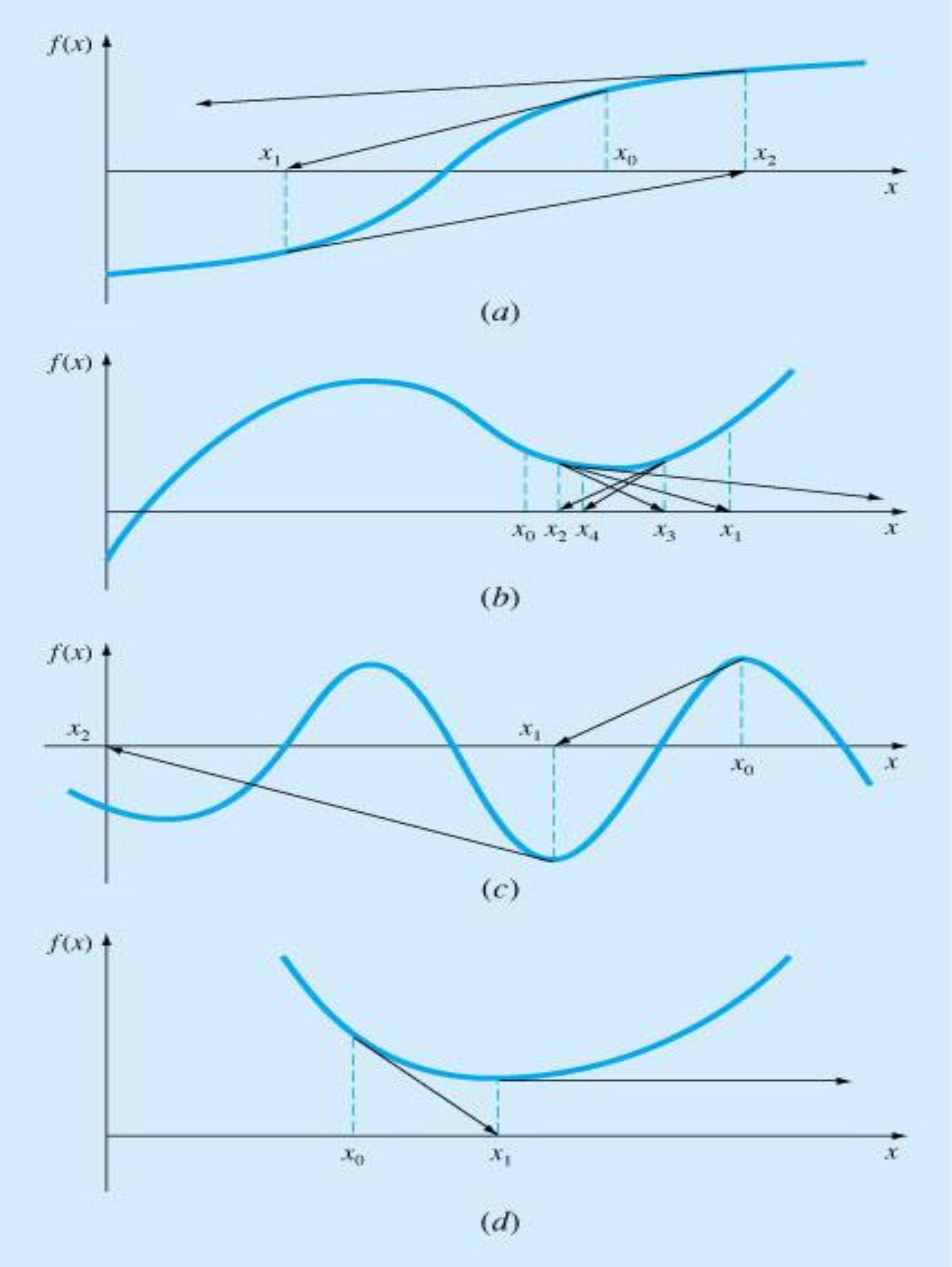
$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

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 $f''(x)$.

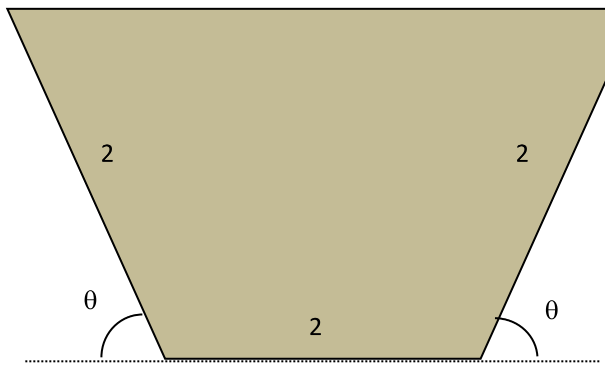
Step 2. Substitute x_i (initial estimate x_0 for the first iteration) $f'(x)$ and $f''(x)$ into

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

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 x_i

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	$f'(\theta)$	$f''(\theta)$	θ *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

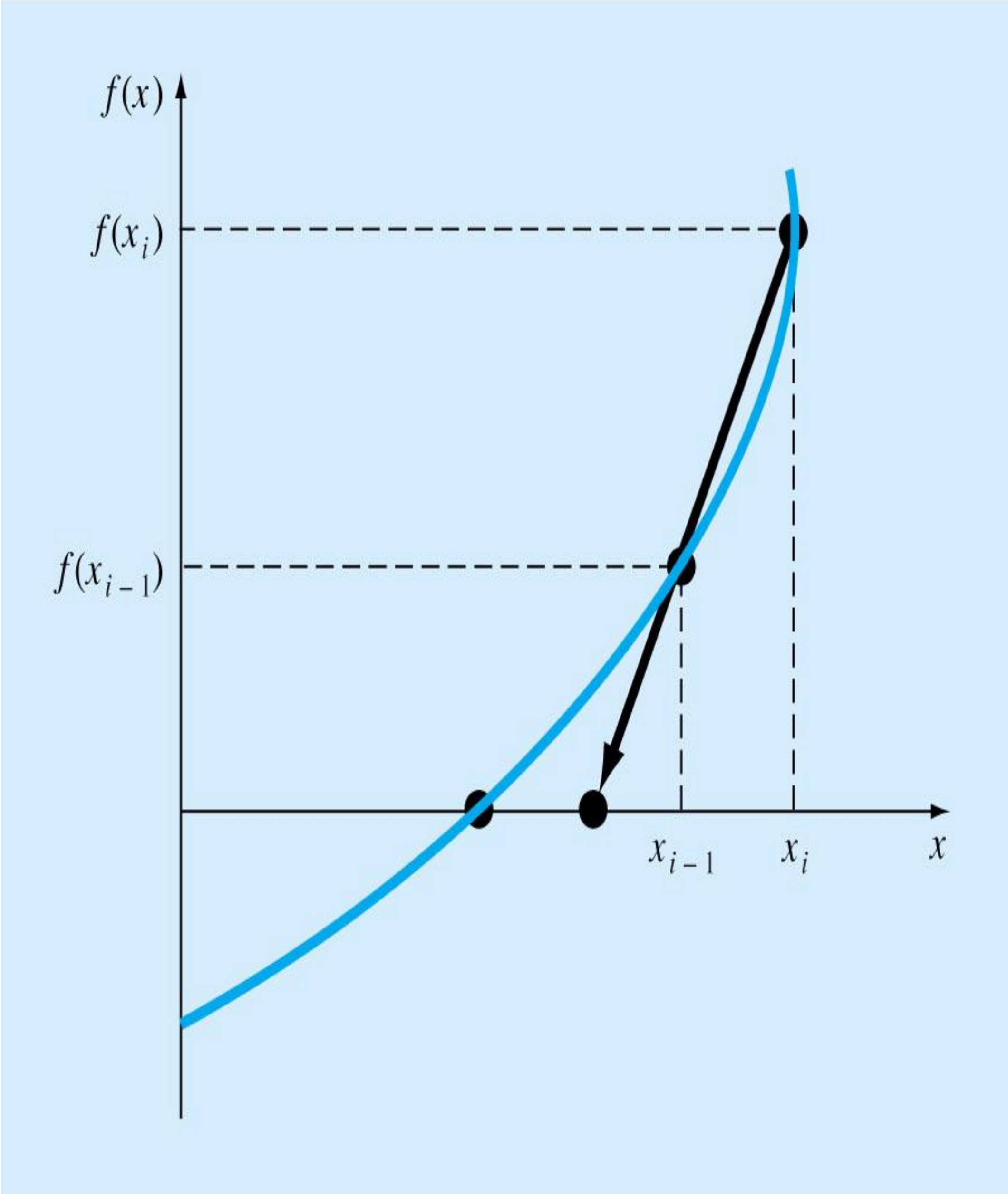
- A slight variation of Newton's method for functions whose derivatives are difficult to evaluate. For these cases the derivative can be approximated by a backward finite divided difference.

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

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

Requires two initial estimates of x , e.g, x_o, 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_o, f(x).



Multidimensional Newton Method

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

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

Taylor Series

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

Jacobian Matrix

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

Iteration function

Multidimensional Newton Method

Computational Aspects

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

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 $F\left(x^k\right), J_F\left(x^k\right)$

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

$k = k + 1$

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

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

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

$$= \begin{bmatrix} 2.000533471 \\ 2.999999894 \end{bmatrix}$$

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

$$= \begin{bmatrix} 2.000000051 \\ 3.000000000 \end{bmatrix}$$

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:

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

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