KMU 255
Computer Programming

Hacettepe University
Department of Chemical Engineering
Fall Semester

Iterative techniques

Selis Önel, PhD

What are we going to learn today?

- Writing codes for iterative solutions
- What are iterative solutions
- When do we need them
- What does the solution look like

Exact Zeros of Nonlinear Algebraic Equations

For a quadratic equation (2nd order polynomial),

Ex: $f(x)=x^2-3$

Exact zeros (roots) of f(x) can be found by the quadratic formula.

- However, no such method exists for most nonlinear functions
- Formula for finding the zeros of a cubic function is very complicated
- Niels Henrik Abel (1802-1829): In 1824 **Abel** proved the impossibility of solving algebraically the general equation of the fifth and higher degrees

Abel, Niels Henrik (1802-1829)

Norwegian mathematician: Born on August 5, 1802 in a small village in Norway

Lived a poor life, caused by large size of his family (6 brothers and father died when he was 18) and difficult economic situation in Norway at that time

Died of tuberculosis at the age of 26 after being forced to live in miserable conditions because of his inability to obtain a university post.

At age 16, gave a proof of the **binomial theorem** valid for all numbers, extending Euler's result which had only held for **rationals**.

At age 19, showed there is no general algebraic solution for the roots of a quintic equation, or any general polynomial equation of degree greater than four, in terms of explicit algebraic operations.

To do this, invented (independently of Galois) an extremely important branch of mathematics known as group theory, which is invaluable not only in many areas of mathematics, but for much of physics as well.

Wrote a monumental work on elliptic functions. However, it was not discovered until after his death.

When asked how he developed his mathematical abilities so rapidly, he replied "**by studying the masters, not their pupils**."

Abel, Niels Henrik (1802-1829)

Abel sent a paper on the unsolvability of the quintic equation to Gauss, who proceeded to discard without a glance what he believed to be the worthless work of a crank.

In 1825, the Norwegian government funded Abel on a scholarly visit to France and Germany. Abel then traveled to Paris, where he gave an important paper revealing the double periodicity of the elliptic functions, which Legendre later described to Cauchy as "a monument more lasting than bronze" (borrowing a famous sentence by the Roman poet Horatius). However, Cauchy proceeded to misplace the manuscript.

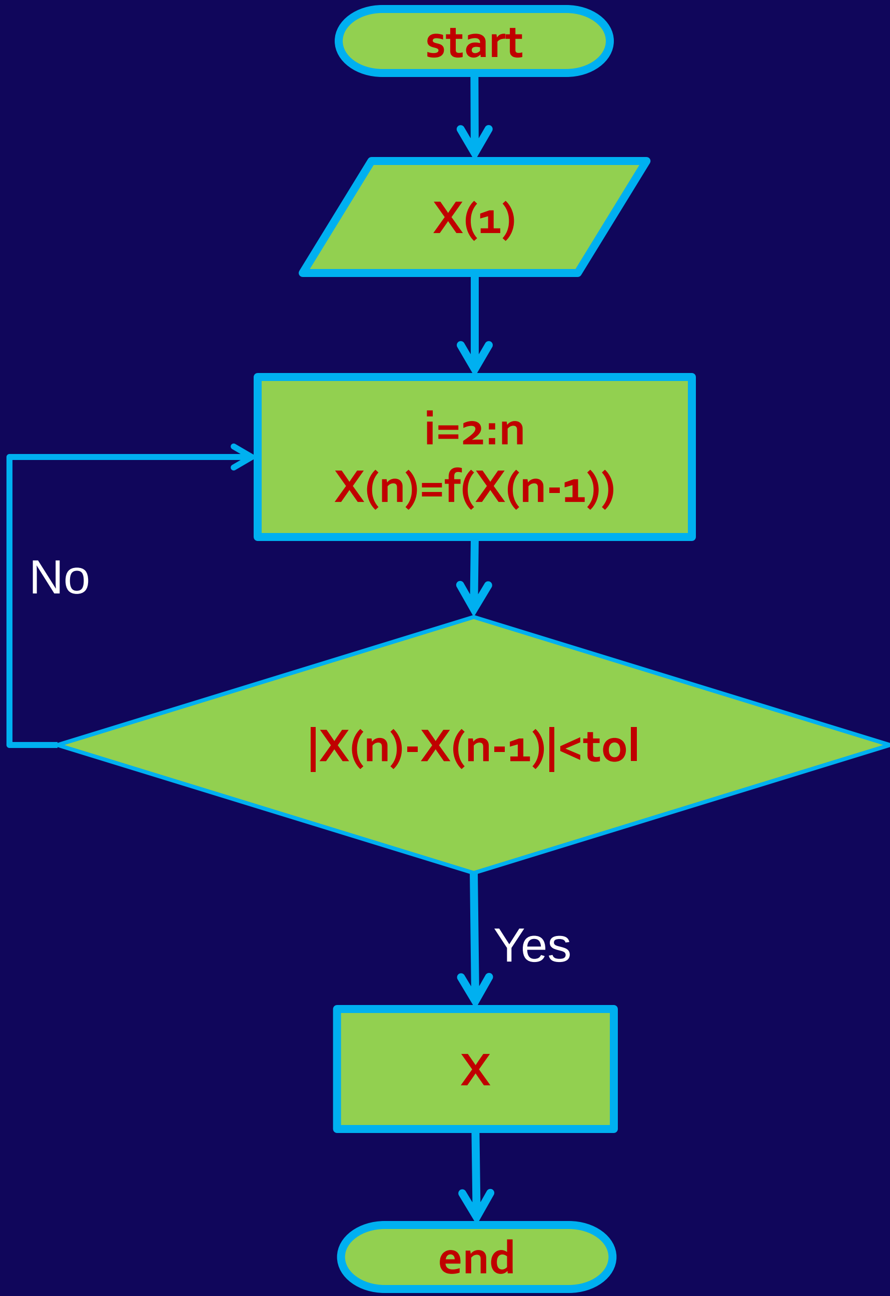
In Berlin, Abel met and was befriended by August Crelle, an amateur mathematician who had founded the famous *Journal für die reine und angewandte Mathematik* (Journal for pure and applied mathematics), which had published several papers by Abel.

However, an offer of a professorship in Berlin was not forthcoming for four years, by which time it was too late. A letter from Crelle arrived two days after Abel's death, informing him that he had been offered professorship at the University of Berlin.

Ref: http://scienceworld.wolfram.com/biography/Abel.html

Iterative methods

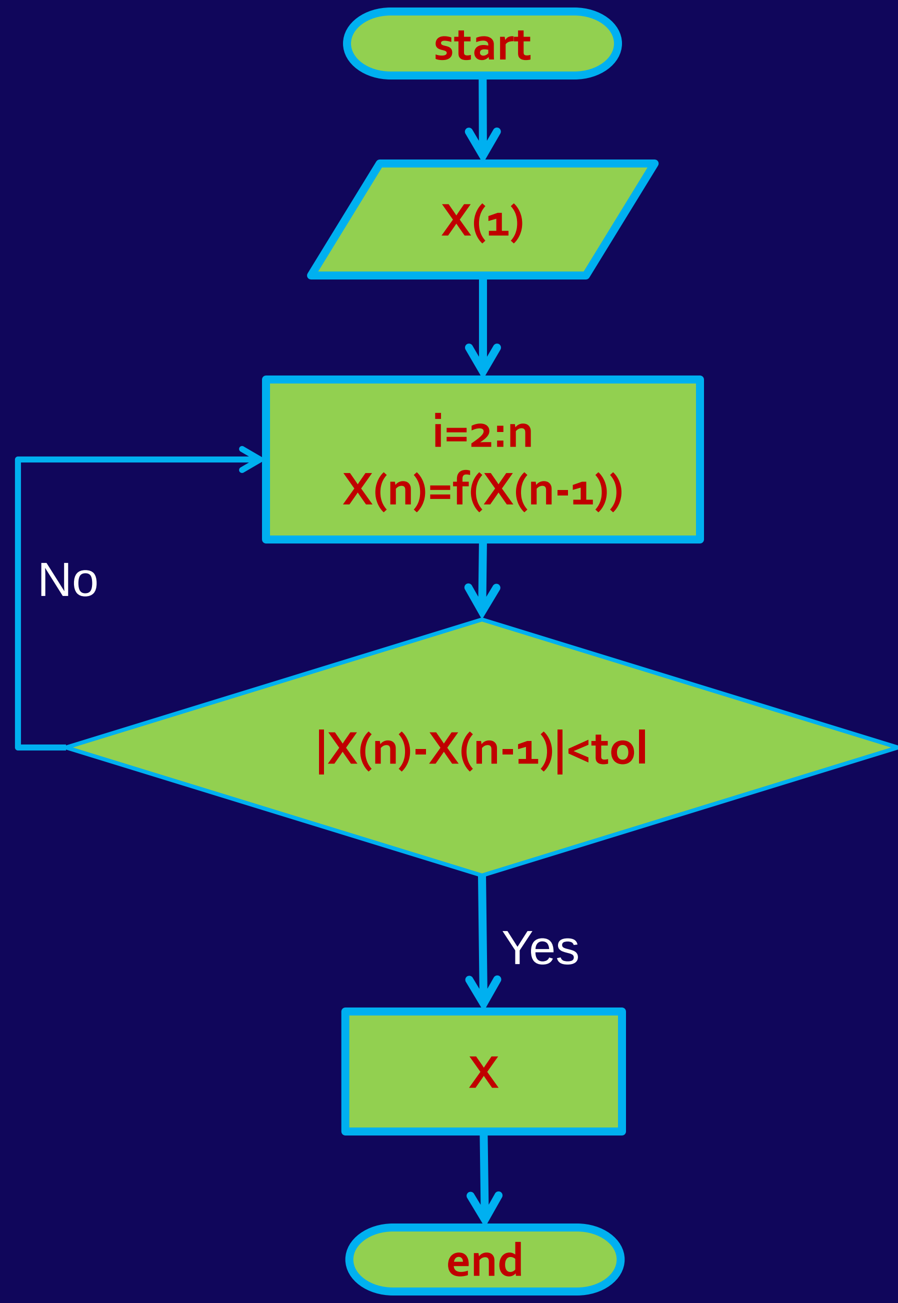
1. Start with approximate answer as the initial guess value, xo
2. Each iteration should improve accuracy
3. Stop once estimated error is below the tolerance value



Iterative methods

are used to find:

1. roots of equations
2. solutions of linear and nonlinear systems of equations
3. solutions of differential equations



Approximate Zeros of a Nonlinear Function using Other Iterative Methods

Fixed point iteration

Bisection method is a systematic searching technique

Secant, false-position and Newton's methods use straight-line approximation to the function whose zero is sought

More powerful methods use a quadratic approximation to the function or a combination of these techniques

Each approach produces a succession of approximations

Choosing the Right Technique

Answer the following questions:

Does the approximation approach the desired solution?

How rapidly is the solution approached?

How much computational effort is required?

Ex: Finding the Square Root Using an Iterative method: Babylonian Method

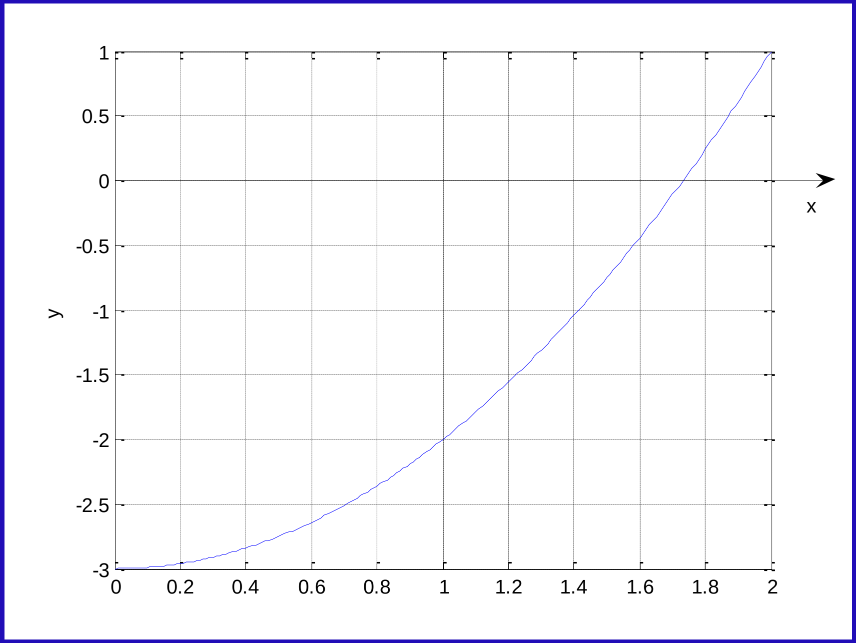
$y=x^2-3$

To find the square root of a positive number c, write $x^2=c$ in implicit form as:

$x=1/2(x+c/x)$

Then use an iterative algorithm to use the RHS of the equation to generate an updated estimate for the desired value of x

```
>> x=0:0.01:2;  y=x.^2-3; plot(x,y);
>> xlabel('x'); ylabel('y'); grid on
```



Babylonian method is a type of "**fixed-point iteration**"

$x_1=1/2(x_0+c/x_0)$

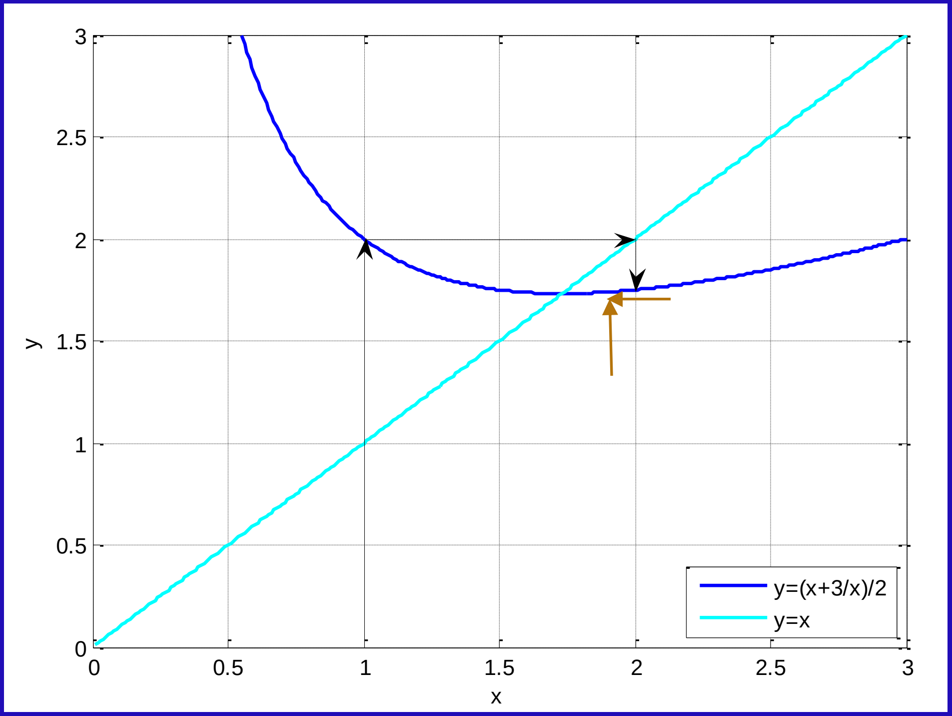
$x_2=1/2(x_1+c/x_1)$

$x_k=1/2(x_{k-1}+c/x_{k-1})$

Ex: Finding the Square Root
Using an Iterative method: Babylonian Method

Fixed point iterations to find a root of $x^2=3$:

```
%Calculate the roots of y=x^2-3, i.e. sqrt(3)
%using fixed point iteration
tol=1;
k=1;
x(k)=1;
while tol>.0001,
   k=k+1;
   x(k)=(x(k-1)+3/x(k-1))/2;
   tol=abs(x(k)-x(k-1));
end
k, x(k), x(k-1)
```



k = 5
x(5) = 1.73205081001473
x(4) = 1.73214285714286
X(3) = 1.75000000000000
X(2) = 2.0

x1=1/2(1+3/1)=2
x2=1/2(2+3/2)=7/4
...
xk=1/2(xk-1+c/xk-1)

Iterative Solution

Good for nonlinear equations or large systems of linear equations when n>>m for $|A_{m,n}||x_{n,1}|= |y_{m,1}|$

(# unknowns is very large compared to # equations)

Simple programming

Applicable to nonlinear coefficients

Requires an initial guess to start the iteration

The goal is to**: (Be Persistent !)**

- Choose a good initial guess xo for x
- Substitute xo in the equations and check if the right hand side of equations is equal to the left hand side or if $x - xo < \varepsilon$
- Increment/decrement xo until all equations are satisfied

Selis Önel, PhD

Quotes of the Day

Nothing in the world can take the place of **Persistence**. Talent will not; nothing is more common than unsuccessful men with talent. Genius will not; unrewarded genius is almost a proverb. Education will not; the world is full of educated derelicts. Persistence and determination alone are omnipotent. The slogan 'Press On' has solved and always will solve the problems of the human race. – *Calvin Coolidge*

Victorious warriors win first and then go to war, while defeated warriors go to war first and then seek to win. – *Sun-Tzu*

Iterative Solutions for linear systems of equations

Popular technique for finding roots of equations

Applied to systems of linear equations to produce accurate results (Generalized ***fixed point iteration***)

Jacobi iteration: Carl Jacobi (1804-1851)

Gauss-Seidel iteration: Johann Carl Friedrich Gauss (1777-1855) and Philipp Ludwig von Seidel (1821-1896)

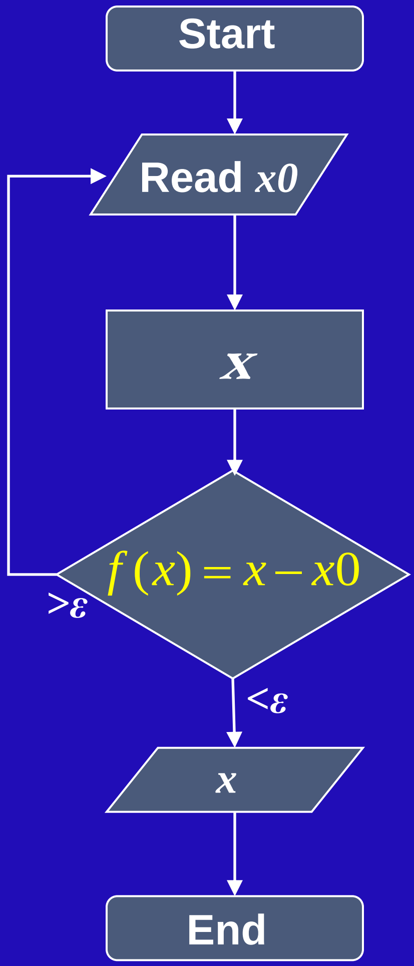
Selis Önel, PhD

Quotations

It is true that Fourier had the opinion that the principal aim of mathematics was public utility and explanation of natural phenomena; but a philosopher like him should have known that the sole end of science is the honor of the human mind, and that under this title a question about numbers is worth as much as a question about the system of the world.
Quoted in N Rose *Mathematical Maxims and Minims* (Raleigh N C 1988). Carl Jacobi

There are problems to whose solution I would attach an infinitely greater importance than to those of mathematics, for example touching ethics, or our relation to God, or concerning our destiny and our future; but their solution lies wholly beyond us and completely outside the province of science.
Quoted in J R Newman, *The World of Mathematics* (New York 1956). Carl Friedrich Gauss

A x = y Solution by Iteration



Input an **initial guess** for iteration to get started

$$x0 = \begin{pmatrix} 0 \\ 0 \\ .. \end{pmatrix}$$

Can be any arbitrary vector xo

Ex: null vector xo=zeros(m,1)

Good **initial guess** →fast **convergence**

Consecutive solution of similar problems: Use the solution of previous problem as the initial guess for the next

Iteration **does not always converge**!

Selis Önel, PhD

A x = y Solution by Iteration: Convergence

Sufficient condition for iteration to converge:

Matrix A should be **diagonally dominant**,

for all i: $$\left|a_{i,i}\right| > \sum_{j=1,\, j\neq i}^{n} \left|a_{i,j}\right|$$ or $$\left|a_{i,i}\right| > \sum_{j=1}^{i-1} \left|a_{i,j}\right| + \sum_{j=i+1}^{n} \left|a_{i,j}\right|$$

i.e. diagonal elements are larger in absolute value than the sum of the absolute value of other coefficients

If a is irreducible (no part of the equation can be solved independently of the rest) for all i

Is it diagonally dominant ?

$$\begin{bmatrix} -2 & 1 & 6 \\ 4 & 7 & 1 \\ 3 & -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 15 \\ -10 \\ 5 \end{bmatrix}$$

- The matrix is <u>NOT</u> diagonally dominant

$$\begin{bmatrix} 3 & -1 & 1 \\ 4 & 7 & 1 \\ -2 & 1 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 5 \\ -10 \\ 15 \end{bmatrix}$$

- The matrix is diagonally dominant

Selis Önel, PhD

A x = y Solution by Iteration: Convergence

The iterative solution described here converges ***unconditionally*** if

for a ***nonsingular matrix***, applied after premultiplying the equation Ax=y by A^t.

$$A^t A x = A^t y$$

Ex: Diagonally Dominant Matrix

Set of equations given by:

(1) $10x_1 - 2x_2 + 5x_3 = 8$

(2) $x_1 + 7x_2 - 3x_3 = 10$

(3) $-4x_1 - 2x_2 - 8x_3 = -20$

is predominantly diagonal as:

$|10|>|-2|+|5|$

$|7|>|1|+|-3|$

$|-8|>|-4|+|-2|$

→

$$Ax = y$$

$$\begin{pmatrix} 10 & -2 & 5 \\ 1 & 7 & -3 \\ -4 & -2 & -8 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 8 \\ 10 \\ -20 \end{pmatrix}$$

Unknown variables on the diagonal are given by:

$$x_1 = \frac{8-(-2x_2+5x_3)}{10}$$

$$x_2 = \frac{10-(x_1-3x_3)}{7}$$

$$x_3 = \frac{-20-(-4x_1-2x_2)}{-8}$$

Ex: Diagonally Dominant Matrix

Given the equations, make a guess starting vector

Solve for x1, x2 and x3 computationally using iteration

→

$$x_1 = \frac{8-(-2x_2+5x_3)}{10}$$

$$x_2 = \frac{10-(x_1-3x_3)}{7}$$

$$x_3 = \frac{-20-(-4x_1-2x_2)}{-8}$$