CUFE, M. Sc., 2015-2016

## Computers \& Numerical Analysis (STR 681)

 Lecture 8 Roots of Nonlinear Equations

Dr. Maha Moddather
Structural Engineering Department
Faculty of Engineering - Cairo University
mahamoddather@eng.cu.edu.eg
Spring 2016

## Introduction

$$
f(x)=a x^{2}+b x+c=0
$$



$$
x=\frac{-b \pm \sqrt{b^{2}-4 a c}}{2 a}
$$

The x's are the roots "zeros" of the equation, meaning?
The values that makes $f(x)$ equals to zero


$$
f(x)=e^{-x}-x \quad \text { Solve? }
$$

## Determining Roots of Equations

- Bracketing Methods.
- Open Methods
- Roots of Polynomials


## Bracketing Methods

- These methods depend on the fact that a function typically changes sign in the vicinity of a root.
- These techniques are called bracketing methods because two initial guesses for the root are required. As the name implies, these guesses must "bracket," or be on either side of, the root.


## Bracketing Methods

## Bracketing Methods include:

$>$ Graphical method.
$>$ Bisection method.
$>$ False position method.
> Incremental searches.

## Graphical Method

- A simple method for obtaining an estimate of the root of the equation $\boldsymbol{f}(\boldsymbol{x})=0$ is to make a plot of the function and observe where it crosses the xaxis.
- This point, which represents the $\boldsymbol{x}$ value for which $\boldsymbol{f}(\boldsymbol{x})=0$, provides a rough approximation of the root.


## Graphical Method

Determine the root for:

$$
f(c)=\frac{667.38}{c}\left(1-e^{-0.146843 c}\right)-40
$$



## Graphical Method

From graph: c = 14.75

$$
\begin{aligned}
f(14.75)=\frac{667.38}{14.75}\left(1-e^{-0.146843(14.75)}\right)-40 & =0.059 \\
& \approx \text { zero }
\end{aligned}
$$



## Graphical Method

- Graphical techniques are of limited practical value because they are not precise. However, graphical methods can be utilized to obtain rough estimates of roots.
- These estimates can be employed as starting guesses for numerical methods discussed later on.
- Graphical interpretations are important tools for understanding the properties of the functions and anticipating the pitfalls of the numerical methods.


## Graphical Method



Between lower bound ( $\mathrm{x}_{\mathrm{I}}$ ) and upper bound $\left(\mathrm{x}_{\mathrm{u}}\right)$ :
(a) Same signs $\rightarrow$ No root

If $f\left(x_{\mathrm{l}}\right)$ and $f\left(\mathrm{x}_{\mathrm{u}}\right)$ have the same sign, there is either no roots or even number of roots.
(b) Same signs $\rightarrow$ Two roots

## Graphical Method



Between lower bound $\left(x_{1}\right)$ and upper bound $\left(\mathrm{x}_{\mathrm{u}}\right)$ :
(c) Opposite signs $\rightarrow$ One root


If $f\left(x_{1}\right)$ and $f\left(x_{u}\right)$ have opposite signs, there are an odd number of roots.
(d) Opposite signs $\quad \rightarrow \quad$ Three roots

## Graphical Method

## Exceptions



Discontinuous equations

## Graphical Method

Use Computer Graphics to locate the roots of equation between $x=4$ and $x=5$ for:

$$
f(x)=\sin 10 x+\cos 3 x
$$

## Graphical Method



## Bisection Method

- If $\boldsymbol{f}(\boldsymbol{x})$ is real and continuous in the interval from $\boldsymbol{x}$, to $\boldsymbol{x}_{\boldsymbol{\mu}}$ and $\boldsymbol{f}(\boldsymbol{x})$ and $\boldsymbol{f}\left(\boldsymbol{x}_{\boldsymbol{L}}\right)$ have opposite signs:

$$
f\left(x_{I}\right) f\left(x_{U}\right)<0
$$

then there is at least one real root between $\boldsymbol{x}$, and $\boldsymbol{x}_{\mu}$ /ncremental search methods capitalize on this observation by locating an interval where the function changes sign. Then the location of the sign change (and consequently, the root) is identified more precisely by dividing the interval into a number of subintervals.

- Each of these subintervals is searched to locate the sign change. The process is repeated and the root estimate refined by dividing the subintervals into finer increments.


## Bisection Method

- The bisection method, which is alternatively called binary chopping or interval halving is one type of incremental search method in which the interval is always divided in half.
- If a function changes sign over an interval, the function value at the midpoint is evaluated.
- The location of the root is then determined as lying at the midpoint of the subinterval within which the sign change occurs. The process is repeated to obtain refined estimates.


## Bisection Method

Step 1: Choose lower $x$ and upper $x_{u}$ guesses for the root such that the function changes sign over the interval. This can be checked by ensuring that $f(x) \mid f\left(x_{0}\right)<0$.

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 $f(x) f\left(x_{r}\right)<0$, the root lies in the lower subinterval. Therefore, set $x_{U}=x_{r}$ and return to step 2.
(b) If $f\left(x_{i}\right) f\left(x_{r}\right)>0$, the root lies in the upper subinterval. Therefore, set $x_{l}=x_{r}$ and return to step 2.
(c) If $f(x) f\left(x_{r}\right)=0$, the root equals $x_{r}$; terminate the computation.

## Bisection Method

- Use Bisection method to locate the roots of equation:

$$
f(c)=\frac{667.38}{c}\left(1-e^{-0.146843 c}\right)-40
$$

- Step 1

Assume $c_{1}=12, c_{u}=16$ (from graphical method)
$f\left(c_{1}\right)=6.06695$
$f\left(c_{u}\right)=-2.26875$

## Bisection Method

- Step 2
$\mathrm{c}_{\mathrm{r}}=\left(\mathrm{c}_{\mathrm{l}}+\mathrm{c}_{\mathrm{u}}\right) / 2=14$
- Step 3
$f\left(c_{r}\right)=1.56871$
$f\left(c_{1}\right) f\left(c_{r}\right)=6.06695 \times 1.56871=9.517285>0$
$\rightarrow$ The root is between $c_{r} \& c_{u}$


## Bisection Method

- Repeat Step 1

Assume $\mathrm{c}_{\mathrm{I}}=14, \mathrm{c}_{\mathrm{u}}=16$
$f\left(\mathrm{c}_{\mathrm{l}}\right)=1.56871 \quad \mathrm{f}\left(\mathrm{c}_{\mathrm{u}}\right)=-2.26875$

- Step 2
$c_{r}=\left(c_{1}+c_{u}\right) / 2=15$
- Step 3
$f\left(c_{r}\right)=-0.42483$
$\mathrm{f}\left(\mathrm{c}_{\mathrm{l}}\right) \mathrm{f}\left(\mathrm{c}_{\mathrm{r}}\right)=1.56871 \times-0.42483=-0.666435<0$
$\rightarrow$ The root is between $c_{r} \& c_{\mid}$(Repeat till accepted error)


## Bisection Method

- Repeat Step 1: $c_{1}=14, c_{u}=15$
- Step 2: $C_{r}=\left(C_{1}+c_{u}\right) / 2=14.5$
- Step 3
$\mathrm{f}\left(\mathrm{c}_{\mathrm{r}}\right)=0.552328 \quad \mathrm{f}\left(\mathrm{c}_{1}\right) \mathrm{f}\left(\mathrm{c}_{\mathrm{r}}\right)=1.56871 \times 0.552328=$ ??????? > 0
$\rightarrow$ The root is between $c_{r} \& c_{u}$ (Repeat till accepted error)

$$
\varepsilon_{a}=\left|\frac{x_{T}^{\text {new }}-x_{r}^{\text {old }}}{x_{r}^{\text {new }}}\right| 100 \% \quad \text { Not the true error!!! }
$$

## Bisection Method

approximate error true (calculable) error

| Iteration | $\mathrm{C}_{\boldsymbol{l}}$ | $\mathrm{C}_{\mathrm{u}}$ | $\mathrm{C}_{\boldsymbol{r}}$ | $\boldsymbol{\varepsilon}_{\boldsymbol{a}}$ (\%) | $\boldsymbol{\varepsilon}_{\boldsymbol{t}}(\%)$ |
| :---: | :--- | :--- | :--- | :--- | :--- |
| 1 | 12 | 16 | 14 |  | 5.279 |
| 2 | 14 | 16 | 15 | 6.667 | 1.487 |
| 3 | 14 | 15 | 14.5 | 3.448 | 1.896 |
| 4 | 14.5 | 15 | 14.75 | 1.695 | 0.204 |
| 5 | 14.75 | 15 | 14.875 | 0.840 | 0.641 |
| 6 | 14.75 | 14.875 | 14.8125 | 0.422 | 0.219 |

True c $\approx 14.7802$

$$
\epsilon_{\mathrm{t}}<\epsilon_{\mathrm{a}}
$$

(conservative)


## False Position Method

- A shortcoming of the bisection method is that, in dividing the interval from $\boldsymbol{x}$, to $\boldsymbol{x}_{\boldsymbol{u}}$ into equal halves, no account is taken of the magnitudes of $\boldsymbol{f}(\boldsymbol{x})$ and $\boldsymbol{f}\left(\boldsymbol{x}_{\boldsymbol{\prime}}\right)$.
- For example, if $\boldsymbol{f}(\boldsymbol{x})$ is much closer to zero than $\boldsymbol{f}\left(\boldsymbol{x}_{\boldsymbol{\psi}}\right)$, it is likely that the root is closer to $\boldsymbol{x}$,than to $\boldsymbol{x}_{\boldsymbol{u}}$



## False Position Method

- An alternative method that exploits this graphical insight is to join $\boldsymbol{f}(\boldsymbol{x})$ and $\boldsymbol{f}\left(\boldsymbol{x}_{\boldsymbol{u}}\right)$ by a straight line.
- The intersection of this line with the $\boldsymbol{x}$ axis represents an improved estimate of the root.
- It is also called the linear interpolation method.

$$
\frac{f\left(x_{I}\right)}{x_{r}-x_{l}}=\frac{f\left(x_{u}\right)}{x_{r}-x_{u}}
$$




## False Position Method

- Use False Position method to locate the roots of equation:

$$
f(c)=\frac{667.38}{c}\left(1-e^{-0.146843 c}\right)-40
$$

## False Position Method

- First Iteration

$$
x_{r}=x_{u}-\frac{f\left(X_{u}\right)\left(x_{I}-x_{u}\right)}{f\left(x_{I}\right)-f\left(X_{u}\right)}
$$

Assume $c_{1}=12, c_{u}=16 \quad$ (from graphical method)
$\mathrm{f}\left(\mathrm{c}_{1}\right)=6.06695$
$f\left(c_{u}\right)=-2.26875$
$c_{r}=16-\left\{\left[-2.26875^{*}(12-16)\right] /[6.06695-(-2.26875)]\right\}=14.9113$

## False Position Method

- Second Iteration

$$
f\left(c_{r}\right)=-0.25426
$$

$$
f\left(c_{\mid}\right) f\left(c_{r}\right)=6.06695 x-0.25426=<0
$$

$\rightarrow$ The root is between $c_{r} \& c_{1}$
Assume $\mathrm{C}_{\mathrm{I}}=12, \mathrm{C}_{\mathrm{u}}=14.9113$
$f\left(\mathrm{c}_{1}\right)=6.06695$
$f\left(c_{u}\right)=-0.25426$
$\mathrm{c}_{\mathrm{r}}=14.9113-\left\{\left[-0.25426^{*}(12-14.9113)\right] /[6.06695-(-0.25426)]\right\}=$ 14.7942

## False Position Method Drawbacks

- Although the false-position method would seem to always be the bracketing method of preference, there are cases where it performs poorly.
- In fact, there are certain cases where bisection yields superior results.
- Use Bisection and False Position methods to locate the roots of equation:

$$
f(x)=x^{10}-1
$$

x is between 0 and 1.3

$$
\text { True answer is } x=1
$$

## False Position Method Drawbacks

- Bisection Method:

| Iteration | $\boldsymbol{x}_{\boldsymbol{I}}$ | $\boldsymbol{x}_{\boldsymbol{u}}$ | $\boldsymbol{x}_{\boldsymbol{r}}$ | $\boldsymbol{\varepsilon}_{\boldsymbol{a}}$ (\%) | $\boldsymbol{\varepsilon}_{\boldsymbol{f}}$ (\%) |
| :---: | :--- | :--- | :--- | :--- | :---: |
| 1 | 0 | 1.3 | 0.65 | 100.0 | 35 |
| 2 | 0.65 | 1.3 | 0.975 | 33.3 | 2.5 |
| 3 | 0.975 | 1.3 | 1.1375 | 14.3 | 13.8 |
| 4 | 0.975 | 1.1375 | 1.05625 | 7.7 | 5.6 |
| 5 | 0.975 | 1.05625 | 1.015625 | 4.0 | 1.6 |

$$
\epsilon_{\mathrm{t}}<\epsilon_{\mathrm{a}}
$$

## False Position Method Drawbacks

- False Position Method:

| Iteration | $\boldsymbol{x}_{\boldsymbol{I}}$ | $\boldsymbol{x}_{\boldsymbol{u}}$ | $\boldsymbol{x}_{\boldsymbol{r}}$ | $\boldsymbol{\varepsilon}_{\boldsymbol{a}}(\%)$ | $\boldsymbol{\varepsilon}_{\boldsymbol{f}}(\%)$ |
| :---: | :--- | :--- | :---: | :---: | :---: |
| 1 | 0 | 1.3 | 0.09430 |  | 90.6 |
| 2 | 0.09430 | 1.3 | 0.18176 | 48.1 | 81.8 |
| 3 | 0.18176 | 1.3 | 0.26287 | 30.9 | 73.7 |
| 4 | 0.26287 | 1.3 | 0.33811 | 22.3 | 66.2 |
| 5 | 0.33811 | 1.3 | 0.40788 | 17.1 | 59.2 |

$$
\epsilon_{\mathrm{t}}>\epsilon_{\mathrm{a}}!!!
$$

## False Position Method Drawbacks

- Slow convergence to solution



## Incremental Searches

- Besides checking an individual answer, you must determine whether all possible roots have been located.
- A plot of the function is usually very useful in guiding you in this task.
- Another option is to incorporate an incremental search at the beginning of the computer program.
- This consists of starting at one end of the region of interest and then making function evaluations at small increments across the region.


## Incremental Searches

- When the function changes sign, it is assumed that a root falls within the increment.
- The $\boldsymbol{x}$ values at the beginning and the end of the increment can then serve as the initial guesses for one of the bracketing techniques.
- A potential problem with an incremental search is the choice of the increment length.


## Incremental Searches

- If the length is too small, the search can be very time consuming.
- On the other hand, if the length is too great, there is a possibility that closely spaced roots might be missed.



## Incremental Searches

- A partial remedy for such cases is to compute the first derivative of the function $f(\boldsymbol{x})$ at the beginning and the end of each interval.
- If the derivative changes sign, it suggests that a minimum or maximum may have occurred and that the interval should be examined more closely for the existence of a possible root.
- You should supplement such automatic techniques with any other information that provides insight into the location of the roots.
- Such information can be found in plotting and in understanding the physical problem from which the equation originated.


## Open Methods

## Open Methods include:

- Simple Fixed-Point Iteration.
- The Newton-Raphson method.
- The Secant method.
- Modified Secant method.
- Multiple roots.
- Systems of Nonlinear equations


## Open Methods

- For the bracketing methods, the root is located within an interval prescribed by a lower and an upper bound.
- Repeated application of these methods always results in closer estimates of the true value of the root.
- Such methods are said to be convergent because they move closer to the truth as the computation progresses.



## Open Methods

- In contrast, the 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.



## Fixed-Point Iteration

- Rearrange the function $\mathrm{f}(\mathrm{x})=0$ so that x is on the left-hand side of the equation:

$$
x=g(x)
$$

- The above equation provides a formula to predict a new value of $\boldsymbol{x}$ as a function of an old value of $\boldsymbol{x}$. Thus, given an initial guess at the root $\boldsymbol{x}_{\boldsymbol{j}}$ to compute a new estimate $\boldsymbol{x}_{\dot{\beta} 1}$ as expressed by the iterative formula:

$$
x_{i+1}=g\left(x_{i}\right)
$$

- As with other iterative formulas in this book, the approximate error for this equation can be determined using the error estimator :

$$
\varepsilon_{a}=\left|\frac{x_{i+1}-x_{i}}{x_{i+1}}\right| 100 \%
$$

## Fixed-Point Iteration

- Use simple fixed-point iteration to locate the root of:

$$
f(x)=e^{-x}-x
$$



$$
x_{i+1}=e^{-x_{i}}
$$

## Fixed-Point Iteration

$$
x_{i+1}=e^{-x_{i}}
$$

- Start with $\mathrm{x}=0$

| $\boldsymbol{i}$ | $\boldsymbol{x}_{\boldsymbol{i}}$ | $\boldsymbol{\varepsilon}_{\boldsymbol{a}}(\%)$ |
| ---: | :---: | :---: |
| 0 | 0 |  |
| 1 | 1.000000 | 100.0 |
| 2 | 0.367879 | 171.8 |
| 3 | 0.692201 | 46.9 |
| 4 | 0.500473 | 38.3 |
| 5 | 0.606244 | 17.4 |
| 6 | 0.545396 | 11.2 |
| 7 | 0.579612 | 5.90 |
| 8 | 0.560115 | 3.48 |
| 9 | 0.571143 | 1.93 |
| 10 | 0.564879 | 1.11 |

## Fixed-Point Iteration

- Convergence occurs only when,

$$
\left|g^{\prime}(x)\right|<1
$$

## Newton-Raphson Method

- The most widely used of all root-locating formulas is the Newton-Raphson equation.
- If the initial guess at the root is $x_{i}$, a tangent can be extended from the point $\left[\mathrm{x}_{\mathrm{i}}, \mathrm{f}\left(\mathrm{x}_{\mathrm{i}}\right)\right]$. The point where this tangent crosses
 the $x$ axis usually represents an improved estimate of the root.

$$
f^{\prime}\left(x_{i}\right)=\frac{f\left(x_{i}\right)-0}{x_{i}-x_{i+1}} \quad \square \quad x_{i+1}=x_{i}-\frac{f\left(x_{i}\right)}{f^{\prime}\left(x_{i}\right)}
$$

## Newton-Raphson Method

- Use Newton-Raphson method to locate the root of:

$$
\begin{gathered}
f(x)=e^{-x}-x \\
\sqrt{b} \\
f^{\prime}(x)=-e^{-x}-1
\end{gathered}
$$


$x_{i+1}=x_{i}-\frac{f\left(x_{i}\right)}{f^{\prime}\left(x_{i}\right)} \Rightarrow x_{i+1}=x_{i}-\frac{e^{-x_{i}}-x_{i}}{-e^{-x_{i}}-1}$

## Newton-Raphson Method

$$
x_{i+1}=x_{i}-\frac{e^{-x_{i}}-x_{i}}{-e^{-x_{i}}-1}
$$

- Start with $\mathrm{x}=0$

| $\boldsymbol{i}$ | $\boldsymbol{x}_{\boldsymbol{i}}$ | $\boldsymbol{\varepsilon}_{\boldsymbol{t}}(\%)$ |
| :--- | :--- | :--- |
| 0 | 0 | 100 |
| 1 | 0.500000000 | 11.8 |
| 2 | 0.566311003 | 0.147 |
| 3 | 0.567143165 | 0.0000220 |
| 4 | 0.567143290 | $<10^{-8}$ |

## Newton-Raphson Method

- Use Newton-Raphson method to locate the root of:

$$
f(x)=x^{10}-1 \quad \text { True answer is } \mathrm{x}=1
$$



$$
f^{\prime}(x)=10 x_{i}^{9}
$$



$$
x_{i+1}=x_{i}-\frac{f\left(x_{i}\right)}{f^{\prime}\left(x_{i}\right)} \Rightarrow x_{i+1}=x_{i}-\frac{x_{i}^{10}-1}{10 x_{i}^{9}}
$$

## Newton-Raphson Method

- Start with $x=0.5$

$$
x_{i+1}=x_{i}-\frac{x_{i}^{10}-1}{10 x_{i}^{9}}
$$

| Iteration | $\boldsymbol{x}$ |
| :---: | :--- |
| 0 | 0.5 |
| 1 | 51.65 |
| 2 | 46.485 |
| 3 | 41.8365 |
| 4 | 37.65285 |
| 5 | 33.887565 |
| $\cdot$ |  |
| $\cdot$ |  |
| $\cdot$ | 1.0000000 |

## Newton-Raphson Method Drawbacks

- An inflection point occurs in the vicinity of a root.

$$
f^{\prime \prime}(x)=0
$$



## Newton-Raphson Method Drawbacks

- The tendency of the Newton-Raphson technique to oscillate around a local maximum or minimum.
- Such oscillations may persist, as a near-zero slope is reached, whereupon the solution is sent far from the area of interest.



## Newton-Raphson Method Drawbacks

- An initial guess that is close to one root can jump to a location several roots away.
- This tendency to move away from the area of interest is because near-zero slopes are encountered.



## Newton-Raphson Method Drawbacks

- A zero slope $\left[f^{\prime}(x)=0\right]$ is truly a disaster because it causes division by zero in the Newton-Raphson formula.
- Graphically, it means that the solution shoots off horizontally and never hits the $x$ axis.



## Newton-Raphson Method Drawbacks

- There is no general convergence criterion for Newton-Raphson. Its convergence depends on the nature of the function and on the accuracy of the initial guess.
- The only remedy is to have an initial guess that is "sufficiently" close to the root.
- Good guesses are usually predicated on knowledge of the physical problem setting or on devices such as graphs that provide insight into the behavior of the solution.
- The lack of a general convergence criterion also suggests that good computer software should be designed to recognize slow convergence or divergence.


## Secant Method

- A potential problem in implementing the Newton-Raphson method is the evaluation of the derivative.
- There are certain functions whose derivatives may be extremely difficult or inconvenient to evaluate.

For these cases, the derivative can
 be approximated by a backward finite divided difference:

$$
f^{\prime}\left(x_{i}\right) \cong \frac{f\left(x_{i-1}\right)-f\left(x_{i}\right)}{x_{i-1}-x_{i}} \square x_{i+1}=x_{i}-\frac{f\left(x_{i}\right)\left(x_{i-1}-x_{i}\right)}{f\left(x_{i-1}\right)-f\left(x_{i}\right)}
$$

## Secant Method

$$
x_{i+1}=x_{i}-\frac{f\left(x_{i}\right)\left(x_{i-1}-x_{i}\right)}{f\left(x_{i-1}\right)-f\left(x_{i}\right)}
$$

- Use secant method to locate the root of, Start with initial estimates of $x_{-1}=0$ and $x_{0}=1.0$ :

$$
f(x)=e^{-x}-x
$$

First iteration:

$$
\begin{aligned}
& x_{-1}=0 \quad f\left(x_{-1}\right)=1.00000 \\
& x_{0}=1 \quad f\left(x_{0}\right)=-0.63212 \\
& x_{1}=1-\frac{-0.63212(0-1)}{1-(-0.63212)}=0.61270
\end{aligned}
$$

## Secant Method

$$
x_{i+1}=x_{i}-\frac{f\left(x_{i}\right)\left(x_{i-1}-x_{i}\right)}{f\left(x_{i-1}\right)-f\left(x_{i}\right)}
$$

Second iteration:

$$
\begin{array}{c|r|}
\begin{array}{l}
x_{0}
\end{array}=1 \\
x_{1}=0.61270 & f\left(x_{0}\right)=-0.63212 \\
f\left(x_{1}\right)=-0.07081
\end{array} \text { both estimates are }
$$

Third iteration:

$$
\begin{array}{ll}
x_{1}=0.61270 & f\left(x_{1}\right)=-0.07081 \\
x_{2}=0.56384 & f\left(x_{2}\right)=0.00518 \\
x_{3}=0.56384-\frac{0.00518(0.61270-0.56384)}{-0.07081-(-0.00518)} & =0.56717
\end{array}
$$

## The difference between Secant \& FalsePosition



False Position


Secant

Both solutions are identical and converge for this iteration !

## The difference between Secant \& FalsePosition



False Position
Still converge


Secant
Can diverge!

## The difference between Secant \& FalsePosition

- Use the false position and secant method to locate the root of, Start with initial estimates of $x_{1}=x_{i-1}=0.5$ and $x_{u}=x_{i}=5.0$ :

$$
f(x)=\ln x \quad \text { True answer is } x=1
$$

False Position

| Iteration | $\boldsymbol{x}_{\boldsymbol{I}}$ | $\boldsymbol{x}_{\boldsymbol{u}}$ | $\boldsymbol{x}_{\boldsymbol{r}}$ |
| :---: | :---: | :--- | :---: |
| 1 | 0.5 | 5.0 | 1.8546 |
| 2 | 0.5 | 1.8546 | 1.2163 |
| 3 | 0.5 | 1.2163 | 1.0585 |

Secant

| Iteration | $\boldsymbol{x}_{\boldsymbol{i}-\mathbf{1}}$ | $\boldsymbol{x}_{\boldsymbol{i}}$ | $\boldsymbol{x}_{\boldsymbol{i}+\boldsymbol{1}}$ |
| :---: | :---: | :--- | :---: |
| 1 | 0.5 | 5.0 | 1.8546 |
| 2 | 5.0 | 1.8546 | -0.10438 |

## Modified Secant Method

- Rather than using two arbitrary values to estimate the derivative, an alternative approach involves a fractional perturbation of the independent variable to estimate $f(x)$.

$$
f^{\prime}\left(x_{i}\right) \cong \frac{f\left(x_{i}+\delta x_{i}\right)-f\left(x_{i}\right)}{\delta x_{i}}
$$

- where $\delta=$ a small perturbation fraction. This approximation can be substituted into previous equation to yield the following iterative equation:

$$
x_{i+1}=x_{i}-\frac{\delta x_{i} f\left(x_{i}\right)}{f\left(x_{i}+\delta x_{i}\right)-f\left(x_{i}\right)}
$$

## Modified Secant Method

- The choice of a proper value for $\delta$ is not automatic. If $\delta$ is too small, the method can be swamped by round-off error caused by subtractive cancellation in the denominator.
- If it is too big, the technique can become inefficient and even divergent.
- However, if chosen correctly, it provides an adequate alternative for cases where evaluating the derivative is difficult and developing two initial guesses is inconvenient.


## Secant Method

$$
x_{i+1}=x_{i}-\frac{\delta x_{i} f\left(x_{i}\right)}{f\left(x_{i}+\delta x_{i}\right)-f\left(x_{i}\right)}
$$

- Use modified secant method to locate the root of, Start initial estimate of $\mathrm{x}_{0}=1.0, \delta=0.01$.

$$
f(x)=e^{-x}-x
$$

First iteration:

$$
\begin{array}{lrl}
x_{0}=1 & f\left(x_{0}\right) & =-0.63212 \\
x_{0}+\delta x_{0}=1.01 & f\left(x_{0}+\delta x_{0}\right) & =-0.64578 \\
& x_{1}=1-\frac{0.01(-0.63212)}{-0.64578-(-0.63212)} & =0.537263
\end{array}
$$

## Secant Method

$$
x_{i+1}=x_{i}-\frac{\delta x_{i} f\left(x_{i}\right)}{f\left(x_{i}+\delta x_{i}\right)-f\left(x_{i}\right)}
$$

Second iteration:

$$
\begin{array}{lr}
x_{0}=0.537263 & f\left(x_{0}\right)=0.047083 \\
x_{0}+\delta x_{0}=0.542635 & f\left(x_{0}+\delta x_{0}\right)=0.038579 \\
x_{1}=0.537263-\frac{0.005373(0.047083)}{0.038579-0.047083}=0.56701
\end{array}
$$

Third iteration:

$$
\begin{array}{lr}
x_{0}=0.56701 & f\left(x_{0}\right)=0.000209 \\
x_{0}+\delta x_{0}=0.572680 \quad f\left(x_{0}+\delta x_{0}\right)=-0.00867 \\
x_{1}=0.56701-\frac{0.00567(0.000209)}{-0.00867-0.000209}=0.567143
\end{array}
$$

## Multiple Roots

- A multiple root corresponds to a point where a function is tangent to the $x$ axis.
- A double root results from The equation has a double root because one value of x makes two terms equal to zero.
- Graphically, this corresponds to the curve touching the x axis tangentially at the double root.

$$
f(x)=x^{3}-5 x^{2}+7 x-3
$$



$$
f(x)=(x-3)(x-1)(x-1)
$$



## Multiple Roots

$$
f(x)=x^{4}-6 x^{3}+12 x^{2}-10 x+3
$$



$$
f(x)=(x-3)(x-1)(x-1)(x-1)
$$



## Multiple Roots

$$
f(x)=(x-3)(x-1)(x-1)(x-1)(x-1)
$$



## Multiple Roots

Multiple roots pose some difficulties for many of the numerical methods:

- The fact that the function does not change sign at even multiple roots precludes the use of the reliable bracketing methods.
- Not only $f(x)$ but also $f^{\prime}(x)$ goes to zero at the root. This poses problems for both the Newton-Raphson and secant methods, which both contain the derivative (or its estimate) in the denominator of their respective formulas. This could result in division by zero when the solution converges very close to the root.


## Modified Newton-Raphson Method

$$
u(x)=\frac{f(x)}{f^{\prime}(x)} \quad \square \quad u^{\prime}(x)=\frac{f^{\prime}(x) f^{\prime}(x)-f(x) f^{\prime \prime}(x)}{\left[f^{\prime}(x)\right]^{2}}
$$



$$
x_{i+1}=x_{i}-\frac{f\left(x_{i}\right) f^{\prime}\left(x_{i}\right)}{\left[f^{\prime}\left(x_{i}\right)\right]^{2}-f\left(x_{i}\right) f^{\prime \prime}\left(x_{i}\right)}
$$

## Modified Newton-Raphson Method

- Use both standard and modified Newton-Raphson to evaluate the multiple root, with an initial guess of $x_{0}=0$.

$$
f(x)=x^{3}-5 x^{2}+7 x-3
$$



$$
f^{\prime}(x)=3 x^{2}-10 x+7
$$



$$
f^{\prime \prime}(x)=6 x-10
$$

## Modified Newton-Raphson Method

Standard

$$
x_{i+1}=x_{i}-\frac{x_{i}^{3}-5 x_{i}^{2}+7 x_{i}-3}{3 x_{i}^{2}-10 x_{i}+7}
$$

$$
x_{i+1}=x_{i}-\frac{\left(x_{i}^{3}-5 x_{i}^{2}+7 x_{i}-3\right)\left(3 x_{i}^{2}-10 x_{i}+7\right)}{\left(3 x_{i}^{2}-10 x_{i}+7\right)^{2}-\left(x_{i}^{3}-5 x_{i}^{2}+7 x_{i}-3\right)\left(6 x_{i}-10\right)}
$$

Modified


## Modified Newton-Raphson Method

$$
\operatorname{Try} x_{0}=2
$$

Standard
$x_{i+1}=x_{i}-\frac{x_{i}^{3}-5 x_{i}^{2}+7 x_{i}-3}{3 x_{i}^{2}-10 x_{i}+7}$

| $\mathbf{i}$ | $\mathrm{x}_{\mathrm{i}}$ |
| :---: | :---: |
| 0 | 2.000000 |
| 1 | 1.000000 |
| 2 | \#DIV/0! |

Modified

$$
x_{i+1}=x_{i}-\frac{\left(x_{i}^{3}-5 x_{i}^{2}+7 x_{i}-3\right)\left(3 x_{i}^{2}-10 x_{i}+7\right)}{\left(3 x_{i}^{2}-10 x_{i}+7\right)^{2}-\left(x_{i}^{3}-5 x_{i}^{2}+7 x_{i}-3\right)\left(6 x_{i}-10\right)}
$$

| $\mathbf{i}$ | $\mathbf{x i}$ |
| :---: | :---: |
| $\mathbf{0}$ | 2.000000 |
| 1 | 1.666667 |
| 2 | 1.222222 |
| 3 | 1.015504 |
| 4 | 1.000061 |
| 5 | 1.000000 |
| 6 | 1.000000 |

## Systems of Nonlinear Equations

$$
\begin{aligned}
& x^{2}+x y=10 \\
& y+3 x y^{2}=57
\end{aligned}
$$



$$
\begin{aligned}
& u(x, y)=x^{2}+x y-10=0 \\
& v(x, y)=y+3 x y^{2}-57=0
\end{aligned}
$$

- The solution would be the values of $x$ and $y$ that make the functions $u(x, y)$ and $v(x, y)$ equal to zero.
- Most approaches for determining such solutions are extensions of the open methods for solving single equations.


## Using Fixed-Point Iteration

- Use fixed-point iteration to determine the roots Initiate the computation with guesses of $\boldsymbol{x}=1.5$ and $\boldsymbol{y}=3.5$

$$
\begin{array}{ll}
x^{2}+x y=10 & \square \\
y+3 x y^{2}=57 & \square \\
y=\sqrt{\frac{57-y}{3 x}}
\end{array}
$$

True answer is $x=2, y=3$

## Using Fixed-Point Iteration

First Iteration

$$
x=\sqrt{10-1.5(3.5)}=2.17945
$$

$$
y=\sqrt{\frac{57-3.5}{3(2.17945)}}=2.86051
$$

Second Iteration

$$
x=\sqrt{10-2.17945(2.86051)}=1.94053
$$

$$
y=\sqrt{\frac{57-2.86051}{3(1.94053)}}=3.04955
$$

Solution is
converging

## Using Fixed-Point Iteration

- Use fixed-point iteration to determine the roots Initiate the computation with guesses of $\boldsymbol{x}=1.5$ and $\boldsymbol{y}=3.5$

$$
\begin{array}{ll}
x^{2}+x y=10 & \square
\end{array} x_{i+1}=\frac{10-x_{i}^{2}}{y_{i}}
$$

True answer is $x=2, y=3$

## Using Fixed-Point Iteration

First Iteration

$$
\begin{aligned}
& x=\frac{10-(1.5)^{2}}{3.5}=2.21429 \\
& y=57-3(2.21429)(3.5)^{2}=-24.37516
\end{aligned}
$$

Second Iteration

$$
\begin{array}{ll}
x=\frac{10-(2.21429)^{2}}{-24.37516}=-0.20910 & \text { Solution is } \\
y=57-3(-0.20910)(-24.37516)^{2}=429.709 & \text { diverging! }
\end{array}
$$

## Using Fixed-Point Iteration

- The most serious shortcoming of simple fixed-point iteration, that convergence often depends on the manner in which the equations are formulated.
- Additionally, even in those instances where convergence is possible, divergence can occur if the initial guesses are insufficiently close to the true solution.


## Using Fixed-Point Iteration

- Sufficient conditions for convergence for the twoequation case are:

$$
\begin{aligned}
& \left|\frac{\partial u}{\partial x}\right|+\left|\frac{\partial u}{\partial y}\right|<1 \\
& \left|\frac{\partial v}{\partial x}\right|+\left|\frac{\partial v}{\partial y}\right|<1
\end{aligned}
$$

- These criteria are so restrictive that fixed-point iteration has limited utility for solving nonlinear systems


## Using Newton-Raphson Method

$$
\begin{aligned}
x_{i+1} & =x_{i}-\frac{u_{i} \frac{\partial v_{i}}{\partial y}-v_{i} \frac{\partial u_{i}}{\partial y}}{\frac{\partial u_{i}}{\partial x} \frac{\partial v_{i}}{\partial y}-\frac{\partial u_{i}}{\partial y} \frac{\partial v_{i}}{\partial x}} \\
y_{i+1} & =y_{i}-\frac{v_{i} \frac{\partial u_{i}}{\partial x}-u_{i} \frac{\partial v_{i}}{\partial x}}{\frac{\partial u_{i}}{\partial x} \frac{\partial v_{i}}{\partial y}-\frac{\partial u_{i}}{\partial y} \frac{\partial v_{i}}{\partial x}}
\end{aligned}
$$

## Using Fixed-Point Iteration

True answer is $x=2, y=3$

- Use Newton-Raphson method to determine the roots Initiate the computation with guesses of $\boldsymbol{x}=1.5$ and $\boldsymbol{y}=$

$$
\begin{aligned}
& x^{2}+x y=10 \\
& y+3 x y^{2}=57
\end{aligned} \quad \square \quad \begin{aligned}
& u(x, y)=x^{2}+x y-10=0 \\
& v(x, y)=y+3 x y^{2}-57=0
\end{aligned}
$$



$$
\begin{array}{ll}
\frac{\partial u_{\square}}{\partial y}=x & \frac{\partial v \square}{\partial x}=3 y^{2} \\
\frac{\partial u_{\square}}{\partial x}=2 x+y & \frac{\partial v_{\square}}{\partial y}=1+6 x y
\end{array}
$$

## Using Fixed-Point Iteration

True answer is $x=2, y=3$
First Iteration

$$
\begin{aligned}
& u_{0}=(1.5)^{2}+1.5(3.5)-10=-2.5 \quad v_{0}=3.5+3(1.5)(3.5)^{2}-57=1.625 \\
& \frac{\partial u_{0}}{\partial x}=2 x+y=2(1.5)+3.5=6.5 \quad \frac{\partial v_{0}}{\partial x}=3 y^{2}=3(3.5)^{2}=36.75 \\
& \frac{\partial u_{0}}{\partial y}=x=1.5 \\
& \frac{\partial v_{0}}{\partial y}=1+6 x y=1+6(1.5)(3.5)=32.5 \\
& \frac{\partial u_{i}}{\partial x} \frac{\partial v_{i}}{\partial y}-\frac{\partial u_{i}}{\partial y} \frac{\partial v_{i}}{\partial x}=6.5(32.5)-1.5(36.75)=156.125 \\
& x=1.5-\frac{-2.5(32.5)-1.625(1.5)}{156.125}=2.03603 \\
& y=3.5-\frac{1.625(6.5)-(-2.5)(36.75)}{156.125}=2.84388
\end{aligned}
$$

## Roots of Polynomials

$$
f_{n}(x)=a_{0}+a_{1} x+a_{2} x^{2}+\cdots+a_{n} x^{n}
$$

The roots of such polynomials follow these rules:

- For an $\boldsymbol{\pi}$ h-order equation, there are $n$ real or complex roots. If $n$ is odd, there is at least one real root.
- If complex roots exist, they exist in conjugate pairs (that is, $\lambda+\mu \dot{\mu}$ and $\lambda-\mu \grave{x}$, where $\dot{\boldsymbol{j}}=\sqrt{ }-1$.

Engineering applications: curve fitting

## Roots of Polynomials

- The efficacy of previous approaches depends on whether the problem being solved involves complex roots.
- If only real roots exist, any of the previously described methods could have utility.
- However, the problem of finding good initial guesses complicates both the bracketing and the open methods, whereas the open methods could be susceptible to divergence.


## Roots of Polynomials

- When complex roots are possible, the bracketing methods cannot be used because of the obvious problem that the criterion for defining a bracket (that is, sign change) does not translate to complex guesses.
- Of the open methods, the conventional Newton-Raphson method would provide a viable approach. However, as might be expected, it would be susceptible to convergence problems.
- For this reason, special methods have been developed to find the real and complex roots of polynomials: The Müller and Bairstow methods.

