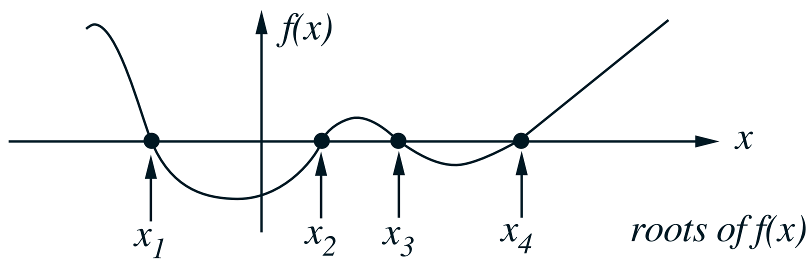
LECTURE 20

SOLVING FOR ROOTS OF NONLINEAR EQUATIONS

• Consider the equation

$$\mathbf{f(x) = 0}$$

• Roots of equation $f(x)$ are the values of x which satisfy the above expression. Also referred to as the zeros of an equation



Example 1

• Find the roots of $f(x) = 3x^5 + 2x^2 + x - 10$

  • Roots of this function are found by examining the equation $3x^5 + 2x^2 + x - 10 = 0$ and solving for the values of x which satisfy this equality.

Example 2

- Solve $\tan kx = x$

$$\tan kx = x \quad \Rightarrow$$

$$\tan kx - x = 0 \quad \Rightarrow$$

$$f(x) = \tan kx - x$$

- Roots are found by examining the equation $\tan kx - x = 0$

Example 3

- Find $\sqrt[3]{8}$

$$x = \sqrt[3]{8} \quad \Rightarrow$$

$$x^3 = 8 \quad \Rightarrow$$

$$x^3 - 8 = 0$$

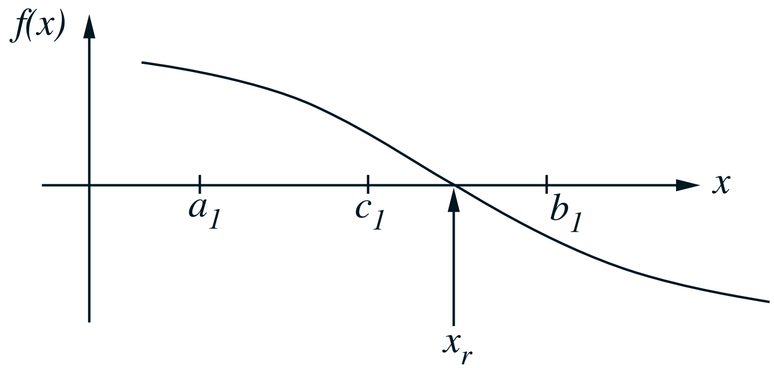
- Find roots by examining the equation $f(x) = x^3 - 8 = 0$.

- Notes on root finding
  - Roots of equations can be either real or complex.
  - Recall $x = a$ is a real number; $x = a + ib$ is a complex number, where $i = \sqrt{-1}$.
  - A large variety of root finding algorithms exist, we will look at only a few.
  - Each algorithm has advantages/disadvantages, possible restrictions, etc.

Method	Must Specify Interval Containing Root	$f^{(1)}(x)$ Continuous	Features
Bisection	yes	no	Robust
Newton-Raphson (Newton)	no	yes	Fast and applies to complex roots

Bisection Method with One Root in a Specified Interval

- You know that the root lies in the interval $[a_1, b_1]$
- x_r = the root that we are looking for

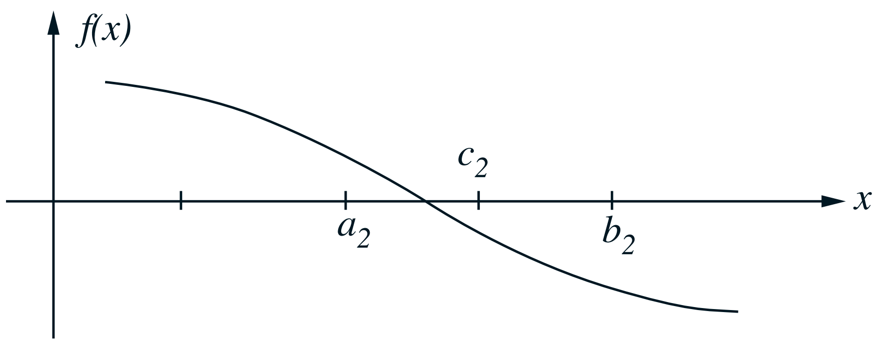


- The midpoint of the starting interval is $c_1 = \dfrac{a_1 + b_1}{2}$
- Evaluate $f(a_1)$, $f(c_1)$, $f(b_1)$. Then consider the product

$$f(a_1)f(c_1) > 0 \quad \Rightarrow \quad \text{root } x_r \text{ must lie in interval } [c_1, b_1]$$

$$f(a_1)f(c_1) \le 0 \quad \Rightarrow \quad \text{root } x_r \text{ must lie in interval } [a_1, c_1]$$

- Selection of the interval is based on the fact that the sign of $f(x)$ changes within the interval in which the root lies.
- Now reset the interval and repeat the process. Therefore for this case, the second iteration interval becomes $[a_2, b_2] = [c_1, b_1]$.
- Now evaluate the midpoint of the second interval as $c_2 = \dfrac{a_2 + b_2}{2}$



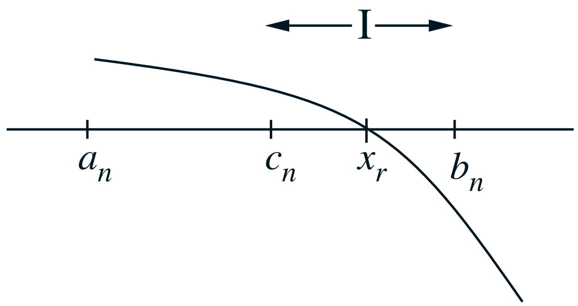
- Evaluate $f(a_2)$, $f(c_2)$, $f(b_2)$. Consider the product

$$f(a_2)f(c_2) > 0 \quad \Rightarrow \text{ root } x_r \text{ must lie in interval } [c_2, b_2]$$

$$f(a_2)f(c_2) \leq 0 \quad \Rightarrow \text{ root } x_r \text{ must lie in interval } [a_2, c_2]$$

- Repeat until a certain level of convergence has been achieved.
  - Interval size, I, after n steps

$$I = \frac{b_n - a_n}{2} = \frac{b_1 - a_1}{2^n}$$



- The interval size at any given iteration also corresponds to the maximum error in x_r, therefore

$$E_n \leq \frac{b_1 - a_1}{2^n}$$

- If you wish to limit the error to ε

$$\varepsilon \geq \frac{b_1 - a_1}{2^n} \qquad \Rightarrow$$

$$2^n \geq \frac{b_1 - a_1}{\varepsilon} \qquad \Rightarrow$$

$$n \geq \frac{\ln\left(\frac{b_1 - a_1}{\varepsilon}\right)}{\ln 2} \qquad \Rightarrow$$

$$\boldsymbol{n \geq 1.443 \ln\left(\frac{b_1 - a_1}{\varepsilon}\right)}$$

- **You must apply n iterations to ensure the ε level of convergence.**

Example 4

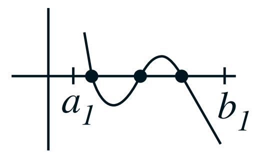
- Find the root of $f(x) = x^2 - 7$ in the interval $[1, 4]$

n Iteration	a_n	b_n	c_n	$f(a_n)$	$f(b_n)$	$f(c_n)$	E_i
1	1	4	2.5	-6	9	-0.75	1.5
2	2.5	4	3.25	-0.75	9	3.56	0.75
3	2.5	3.25	2.875	-0.75	3.56	1.266	0.375
4	2.5	2.875	2.6875	-0.75	1.266	0.2226	0.1875
5	2.5	2.6875	2.59375	-0.75	0.226	-0.27246	0.0937
6	2.59375	2.6875	2.640625 ± 0.0468				0.0468

- The actual root to this equation is 2.645751. The actual error for our 6th iteration estimate is 0.0051.

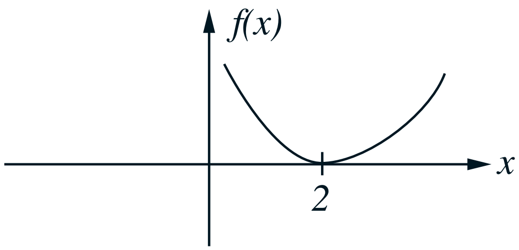
Problems with the Bisection Method

- Multiple roots in an interval $[a_1, b_1]$.



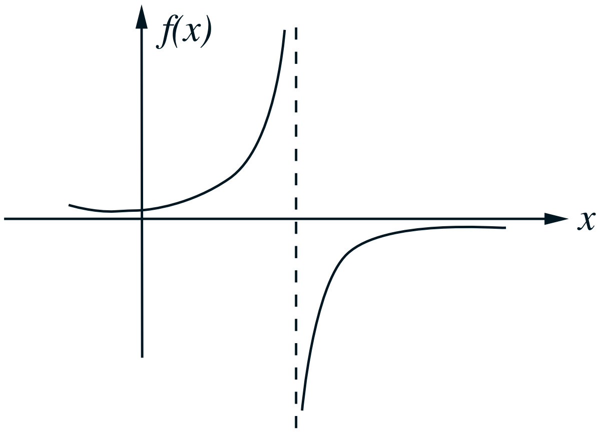
  - If $f(a_1)\ f(b_1) < 0$, then the bisection method will find one of the roots. However it is not very useful to know only one root!
  - Either use another method or provide better intervals. You can use graphical methods or tables to find intervals.

- Double roots



  - The bisection method will not work since the function does not change sign
  - e.g. $f(x) = (x-2)^2$

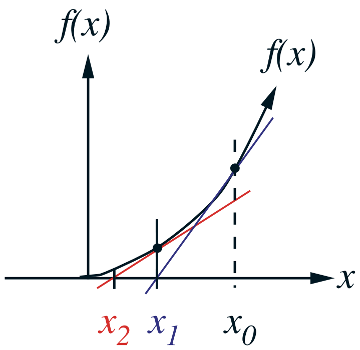
- Singularities



- The bisection method will solve for a singularity as if it were a root. Therefore we must check the functional values to ensure convergence to see if it is indeed a root.

Newton-Raphson Method (a.k.a. Newton Method)

- Finds the root if an initial estimate of the root is known
- Method may be applied to find complex roots
- Method uses a truncated Taylor Series expansion to find the root
- Basic Concept
  - Slope is known at an estimate of the root x_o.
  - Compute the slope of $f(x)$ at the estimate of the root, x_o, and project this slope back to where it crosses the x-axis to find a better estimate for the root.



Derivation of the Newton-Raphson Method

- We want to solve the equation $f(x_r) = 0$

- Taylor series expand $f(x)$ about a point x_o where x_o is an estimate of the root

$$f(x_r) = f(x_o) + f^{(1)}(x_o)(x_r - x_o) + f^{(2)}(\xi)\frac{(x_r - x_o)^2}{2!} \qquad x_o < \xi < x_r$$

  - Explicitly consider terms up to $O(x_r - x_o)$.

  - $O(x_r - x_o)^2$ and higher order terms are ***not*** explicitly accounted for but are represented by the last term in the series and are used to estimate the error.

- Set the series approximation to $f(x_r)$ equal to zero and solve for x_r

$$f(x_o) + f^{(1)}(x_o)(x_r - x_o) + f^{(2)}(\xi)\frac{(x_r - x_o)^2}{2!} = 0 \qquad \Rightarrow$$

$$\boldsymbol{x_r = x_o - \frac{f(x_o)}{f^{(1)}(x_o)} + E} \quad \text{where} \quad \boldsymbol{E = -\frac{f^{(2)}(\xi)}{f^{(1)}(x_o)}\ \frac{(x_r - x_o)^2}{2!}}$$

- The error can be estimated as:

$$E \cong -\frac{f^{(2)}(x_o)}{f^{(1)}(x_o)} \frac{(x_r - x_o)^2}{2!}$$

- We can iteratively update our estimate of x_o with our most recently computed value

$$\boldsymbol{x_n = x_{n-1} - \frac{f(x_{n-1})}{f^{(1)}(x_{n-1})} + E_n}$$

- The error is equal to

$$\boldsymbol{E_n \cong -\frac{f^{(2)}(x_{n-1})}{f^{(1)}(x_{n-1})} \frac{(x_n - x_{n-1})^2}{2!}}$$

  - Note that E_n is not included to update x_n but serves only as an estimate of the error.

Example 5

- Find the root of $f(x) = x^2 - 7$ using an initial estimate $x_0 = 4$

$$x_n = x_{n-1} - \frac{f(x_{n-1})}{f^{(1)}(x_{n-1})} \qquad E_n = -\frac{f^{(2)}(x_{n-1})}{f^{(1)}(x_{n-1})}\frac{(x_n - x_{n-1})^2}{2}$$

$$f^{(1)}(x) = 2x \qquad f^{(2)}(x) = 2$$

n	x_{n-1}	$f(x_{n-1})$	$f^{(1)}(x_{n-1})$	$f^{(2)}(x_{n-1})$	x_n	E_n	E_{actual}
1	4	9	8	2	2.87500	0.1582	0.22924
2	2.87500	1.2656	5.7500	2	2.654891	0.00843	0.00913
3	2.654891	0.04844	5.30978	2	2.645767	0.000015	0.0000157
4	2.645767	0.0000832	5.291534	2	2.64575131	4.6×10^{-11}	-

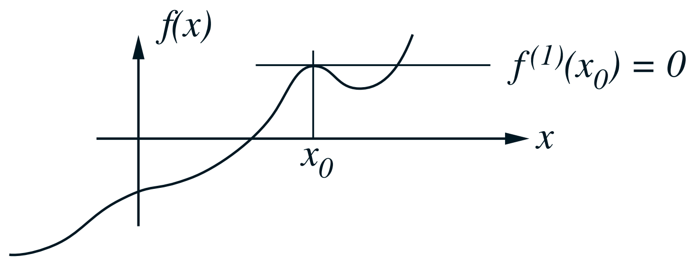
- $x_4^2 - 7 = 0.0000000000$ (up to round-off accuracy of calculator).

Notes on Newton's Method

- Convergence rate for Newton's method is ***very high***!!
- Error estimates are very good (however will be case dependent on the form of the function $f(x)$).
- Newton's method can find complex roots.

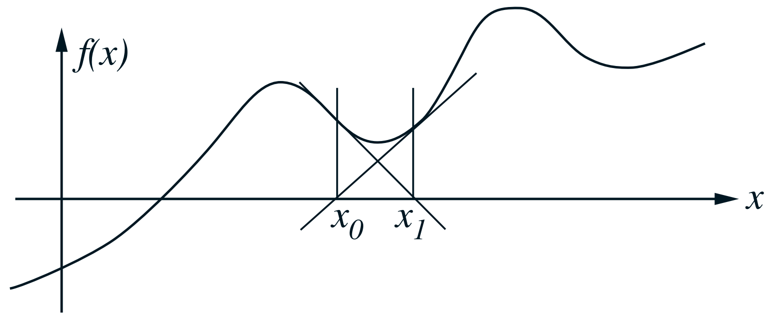
Problems with Newton's Method

- If the local min/max is selected as an initial guess

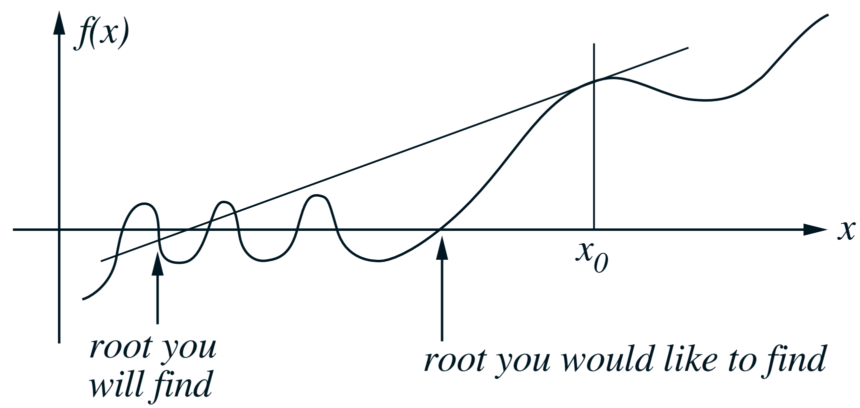


- The slope at x_o does not intersect with x-axis!
- The formula for x_1 will lead to an infinite value.

- If the initial guess is poor (what is poor depends on shape of $f(x)$)
  - The solution may diverge:



  - The solution may converge to another root:



  - Therefore what is a good initial guess depends on the function and how it behaves.

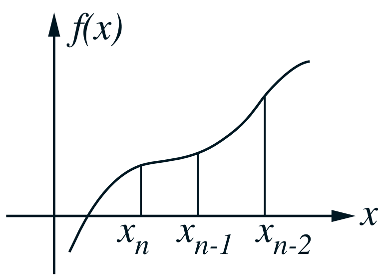
Secant Method

- For cases where it is difficult or expensive to evaluate the first derivative, we can apply the Newton Method using a difference approximation to evaluate the derivative
  - Forward difference approximation $\rightarrow$ *difficult to apply since x_n is included*

$$f^{(1)}(x_{n-1}) = \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}} + O(x_n - x_{n-1})$$

  - Backward difference approximation $\rightarrow$ *readily applied*

$$f^{(1)}(x_{n-1}) = \frac{f(x_{n-2}) - f(x_{n-1})}{x_{n-2} - x_{n-1}} + O(x_{n-2} - x_{n-1})$$



- Applying a backward approximation, the ***Secant*** algorithm to find the root becomes:

$$\boldsymbol{x_n = x_{n-1} - \frac{f(x_{n-1})}{f(x_{n-2}) - f(x_{n-1})}(x_{n-2} - x_{n-1})}$$

SUMMARY OF LECTURE 20

- There are many methods available to find roots of equations
- The Bisection method is a crude but simple method. It is based on the fact that the sign of a function changes in the vicinity of a root. Therefore given an interval within which the root lies, we can narrow down that interval, by examining the sign of the function at the endpoints and midpoint of the interval (i.e. deciding if the sign change in the function occurs on the left half of the interval or the right half.)
- Newton-Raphson is based on using an initial guess for the root and finding the intersection with the axis of the straight line which represents the slope at the initial guess. It works very fast and converges assuming the initial guess was good.
- Very crude methods may have to be used to come up with intervals or initial guesses for roots.
    - Brute force evaluations of functions noting sign changes (even with some iterative refinement in the vicinity of a root/roots)
    - Graphics