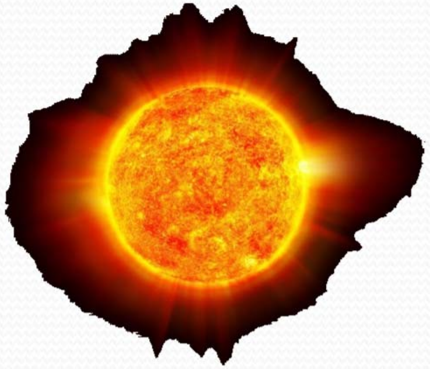
Finding Roots of an equation of a single variable

Computational Physics: R. Landau et. al. Chap. 7
BCCP: B.A. Stickler et al. Appendix B

Finding Lagrange Points of the Earth for Satellite

- Spacecraft that study the Sun are often placed at the so-called L1 Lagrange point, located sunward of Earth on the Sun-Earth line.
- L1 is the point where Earth's and Sun's gravity together produce an orbital period of one year, so that a spacecraft at L1 stays fixed relative to Earth as both planet and spacecraft orbit the Sun.
- Find L1's location relative to Earth.



Problem (I)

- We have a cannon that can fire projectiles with speed v at an angle θ. Question: What angle θ should we use to force our cannon to hit a target a distance R away?

- How to throw a 3pt field goal (6.24m/3.1m)?

Finding Roots

- A very fundamental question in mathematics
- Linear equation, Quadratic Equation,...

$$3x-2=0;$$
$$2x^2-3x+1=0;$$
$$x^5=3;$$
$$(x-3)(x^2-2x+5)=0;$$
$$2x^5-3x+1=0;$$

$$2x^5-5x+1=0;$$
$$x-\cos x=0;$$
$$e^x-x-1=0;$$
$$\frac{1}{x}=\sin 2x$$

Finding Roots

- A closed-form formula of the solutions!?
  - Only up to 4th order polynomial
  - For higher order polynomials, there is no closed form formula

- Roots of a polynomial has been profoundly investigated
  - 代數基本定理與他的好朋友們(除法原理，根與係數關係，...)

- Real roots of a general non-linear equation

Finding Roots

- Pictorial Solution

- Numerical Solutions
  - Can approach root finding problem to all orders

- Programmatic Thinking

Finding Roots

- If you have no idea where the root is
  - Plot out the function

- If you know where a root might be
  - Carefully choose an initial guess

- If you already got a root
  - use what you learned to find other roots.

Finding Roots

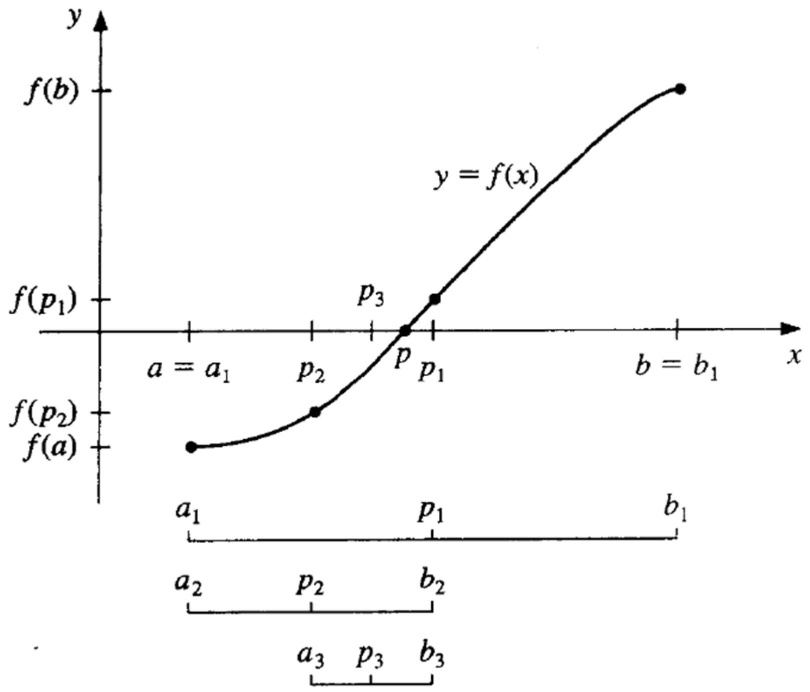
- Bisection Method (Multi-partition Method)
- Fixed Point Method
- Newton-Raphson Method
  - Modified N-R Method
  - Secant Method
- Finding roots for a polynomial function
  - Deflation
  - Muller's Method

Bisection Method

Intermediate Value Theorem

- Suppose f is a continuous function on the interval [a, b]
- f(a) and f(b) have different sign. f(a)*f(b)<o
- There must be at least one root of f within the interval [a,b]

Bisection Method



Bisection Method

- When to stop?
- Setting the error tolerance
- To achieve certain precision
  - If p is away from o

$$\frac{|p_n - p_{n-1}|}{|p_n|} < \varepsilon$$

  - If p is close to o

$$|p_n - p_{n-1}| < \varepsilon$$

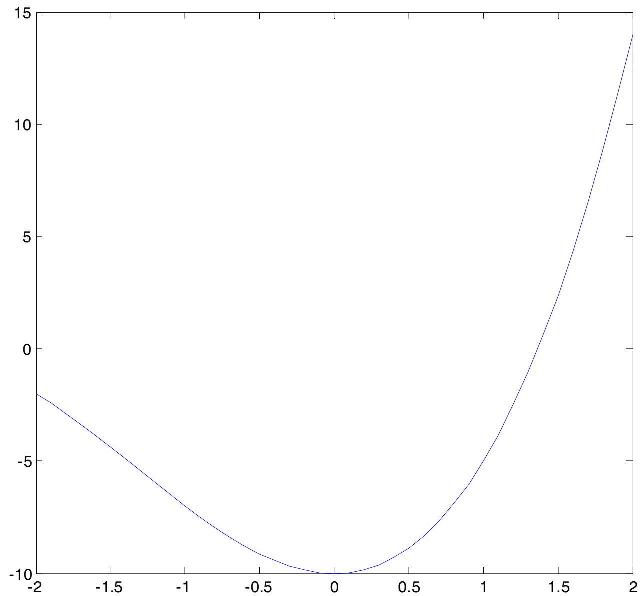
  - Directly test the result

$$f(p_n) < \varepsilon$$

Example

- Solve $$f(x) = x^3 + 4x^2 - 10$$

- First plot the function



Example

- Pick up first 2 guesses [1,2]
  - f(1)=-5 ; f(2)= 14
- Evaluate f(1.5)=2.375
- Replace 2 by 1.5 as they have the same signs
- Keep on the iteration until stop criteria is satisfied.

Example

n	a	b	p	f(a)	f(b)	f(p)
1	1	2	1.5	-5	14	2.375
2	1	1.5	1.25	-5	2.375	-1.79688
3	1.25	1.5	1.375	-1.79688	2.375	0.162109
4	1.25	1.375	1.3125	-1.79688	0.162109	-0.84839
5	1.3125	1.375	1.34375	-0.84839	0.162109	-0.35098
6	1.34375	1.375	1.359375	-0.35098	0.162109	-0.09641
7	1.359375	1.375	1.367188	-0.09641	0.162109	0.032356
8	1.359375	1.367188	1.363281	-0.09641	0.032356	-0.03215
9	1.363281	1.367188	1.365234	-0.03215	0.032356	7.2E-05
10	1.363281	1.365234	1.364258	-0.03215	7.2E-05	-0.01605
11	1.364258	1.365234	1.364746	-0.01605	7.2E-05	-0.00799

Example

- Find a positive root of

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

Bisection Method

- The sequence $\{p_n\}$ that bisection method generates has the following property

$$\left|p_n - p\right| \le \frac{b-a}{2^n}$$

- Based on this property, the number of iterations to achieve final goal can be estimated

Example

- Find the necessary number of iterations to solve

$$f(x) = x^3 + 4x^2 - 10$$

within accuracy 10^{-3} using [1,2] as an initial guess

$$x_c = 1.36523$$

Example

- Check the error bound
- Then
$$|p_n - p| \le \frac{b-a}{2^n}$$

$$|p_n - p| \le \frac{2-1}{2^n} \le 10^{-3}$$

$$n \ge \log_2 10^3 \approx 9.96$$

Example

n	a	b	p	f(a)	f(b)	f(p)
1	1	2	1.5	-5	14	2.375
2	1	1.5	1.25	-5	2.375	-1.79688
3	1.25	1.5	1.375	-1.79688	2.375	0.162109
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Bisection Method

- Based on Intermediate value theorem to systematically search root within a specified interval

- The convergence rate can be expressed as follows

$$\left| p_n - p \right| \le \frac{b-a}{2^n}$$

Multiple Partition method

- The error bound means the maximum distance of interval

$$|p_n - p| \le \frac{b-a}{2^n}$$

- Increase the partition to make the convergence faster
  - 二分逼近法，三分逼近法，… ，十分逼近法，…

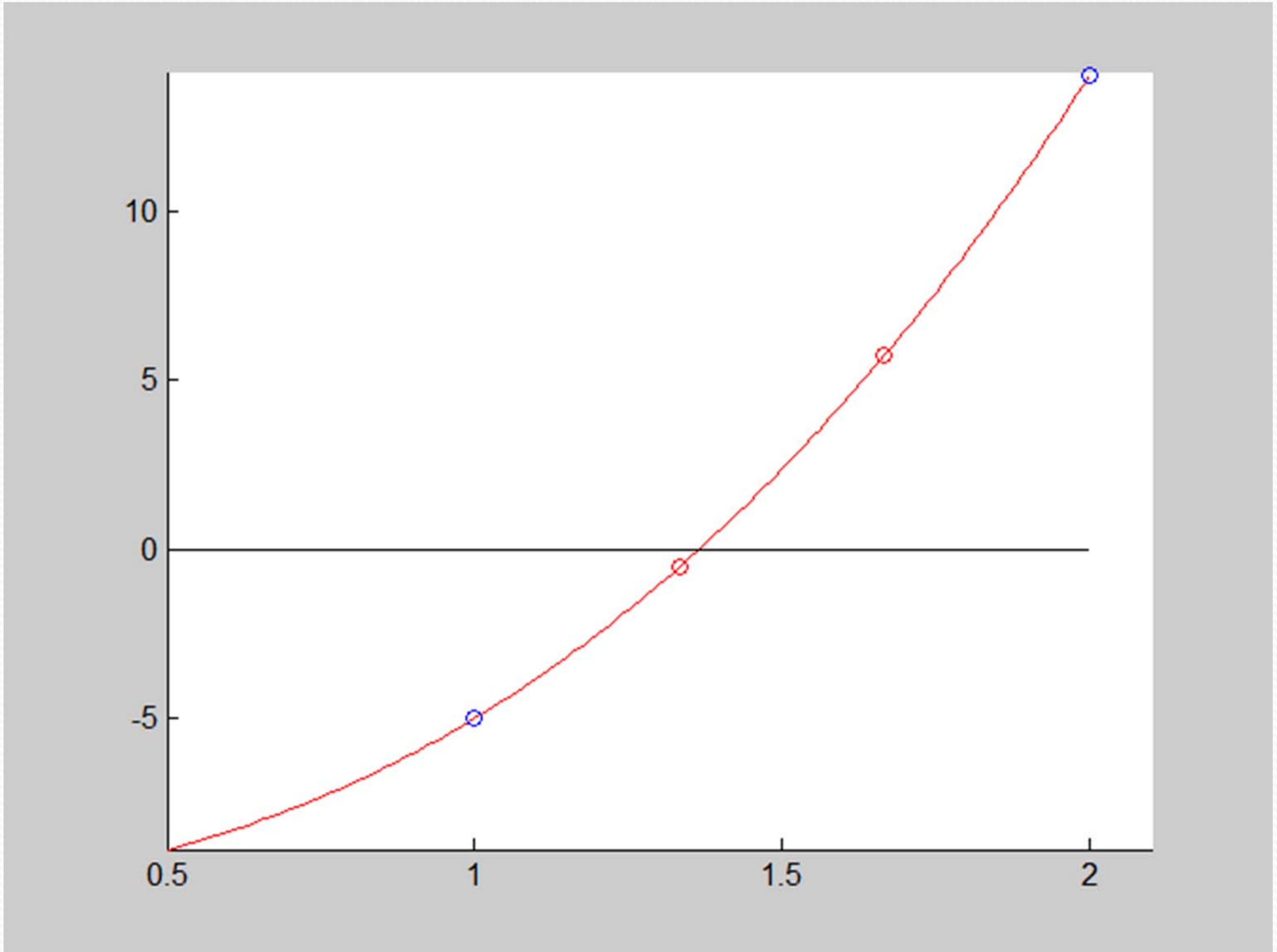
- More evaluation of functions and conditions will be needed

Trisection Method

- Pick up one initial interval [a,b]
  - f(a) ; f(b)
- Evaluate the trisection points

  $f(a + (a-b)/3)$ and $f(a + 2*(a-b)/3)$
- Now you have 3 subsections
- Pick up the section that satisfies Intermediate Value Theorem
- Keep on the iteration until stop criteria satisfied.

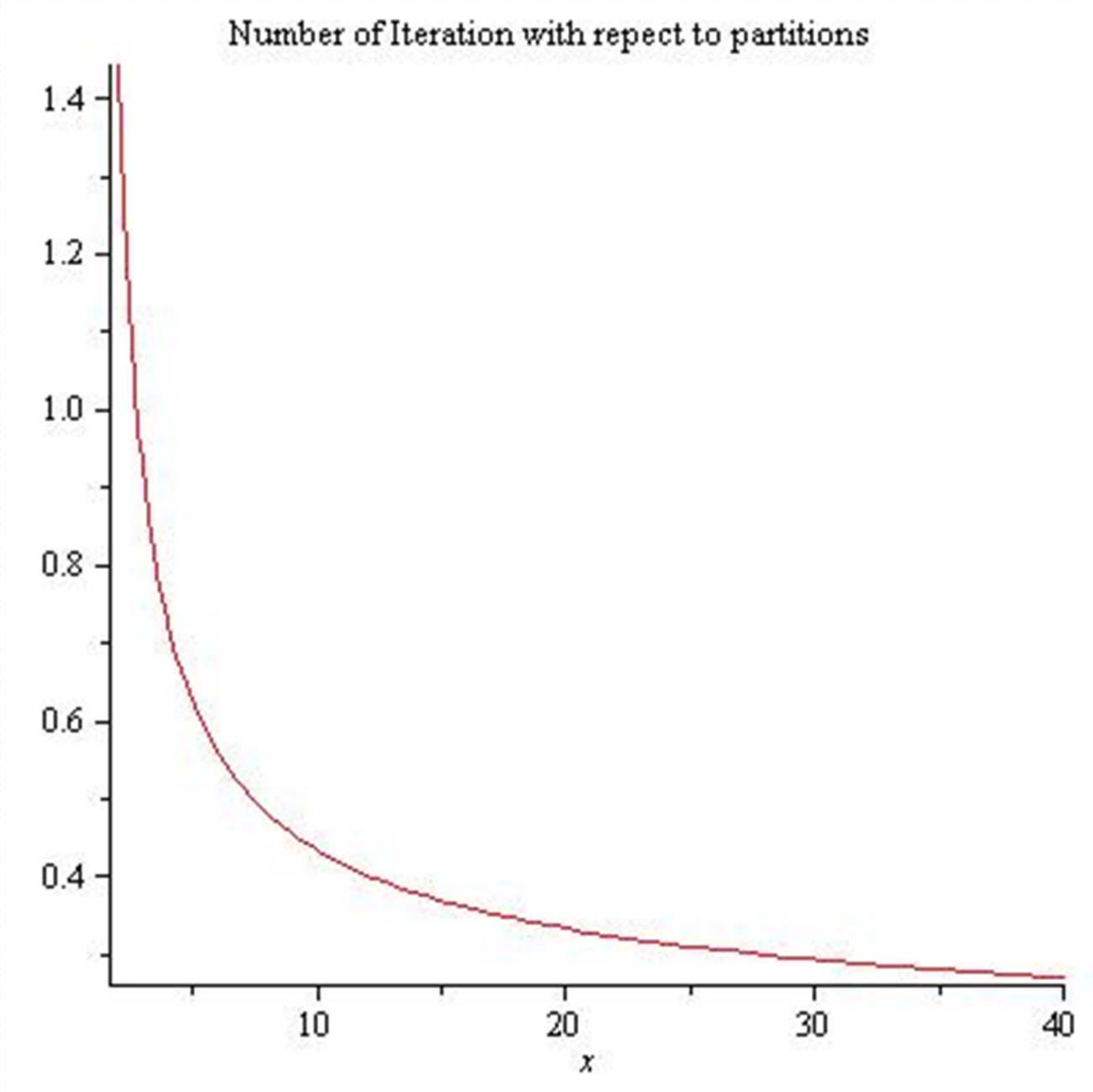
Example



Example

n	a	p1	p2	b	f(a)	f(p1)	f(p2)	f(b)
1	1.00000	1.33333	1.66667	2.00000	-5.00000	-0.51852	5.74074	14.00000
2	1.33333	1.44444	1.55556	1.66667	-0.51852	1.35940	3.44307	5.74074
3	1.33333	1.37037	1.40741	1.44444	-0.51852	0.08510	0.71097	1.35940
4	1.33333	1.34568	1.35802	1.37037	-0.51852	-0.31977	-0.11856	0.08510
5	1.35802	1.36214	1.36626	1.37037	-0.11856	-0.05095	0.01694	0.08510
6	1.36214	1.36351	1.36488	1.36626	-0.05095	-0.02835	-0.00572	0.01694
7	1.36488	1.36534	1.36580	1.36626	-0.00572	0.00183	0.00938	0.01694
8	1.3648834	1.365036	1.365188	1.365341	-0.00572	-0.003207	-0.00069	0.001827
9	1.3651882	1.365239	1.36529	1.365341	-0.00069	0.000149	0.000988	0.001827
10	1.3651882	1.365205	1.365222	1.365239	-0.00069	-0.00041	-0.00013	0.000149

Other Partition method



Fixed Point

Modify the equation to become a fixed point problem.

Fixed Point

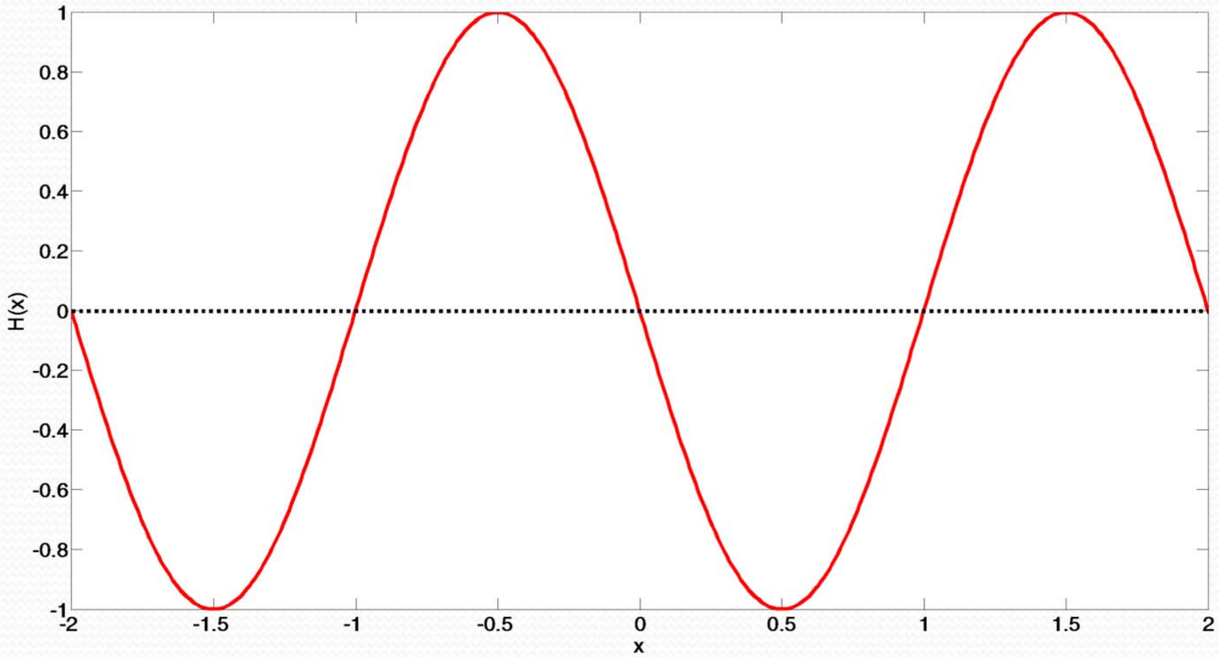
- A fixed point of a given function is a number p that satisfies the following equation.

$$g(p) = p$$

- The intersect of the function g(x) with f(x)=x;
- Also a root of x = g(x);

An Example of Fixed point solver

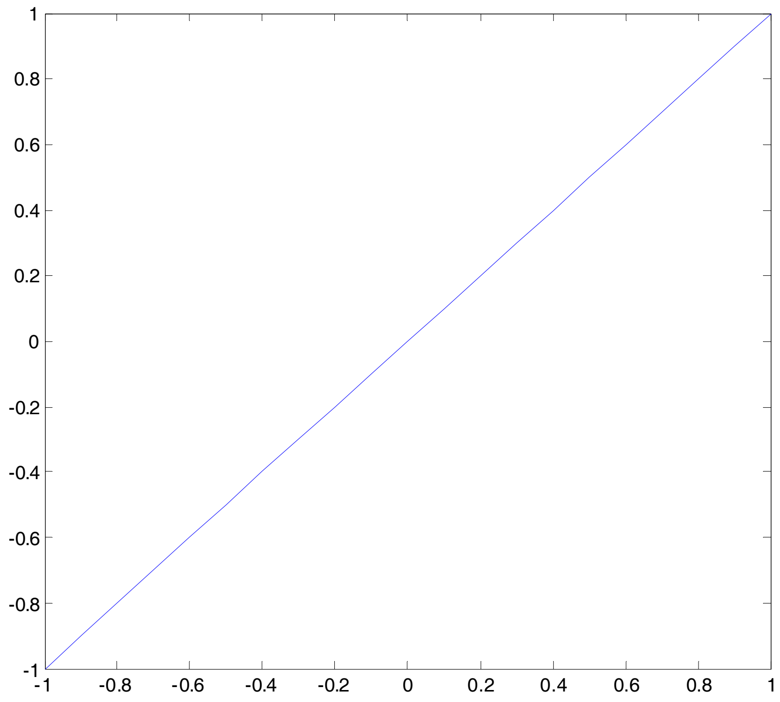
- Find the roots of $H(x) = -\sin \pi x$

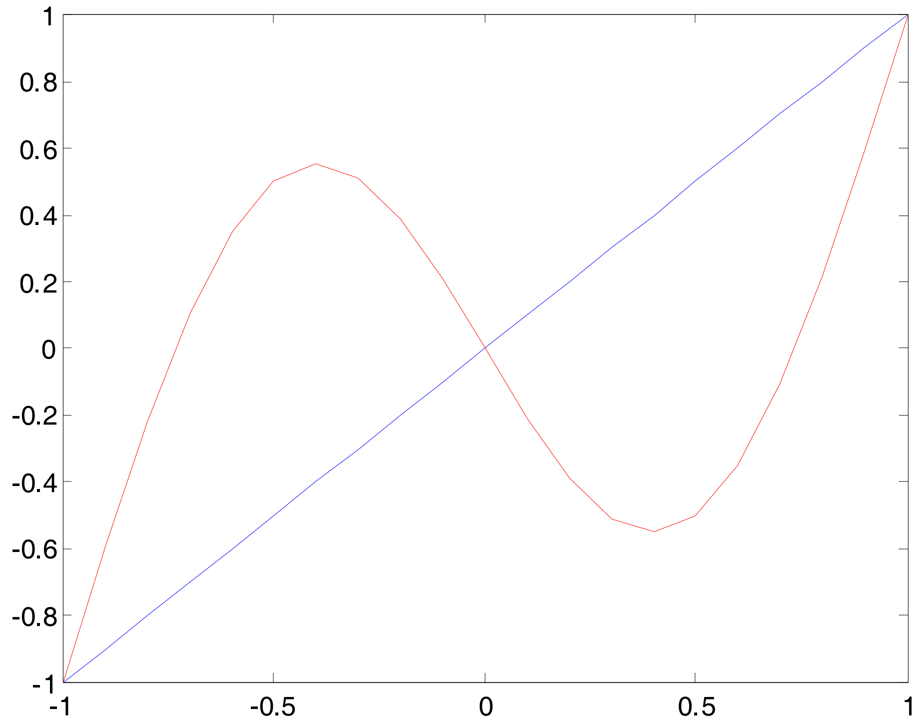


Examples of Fixed Point

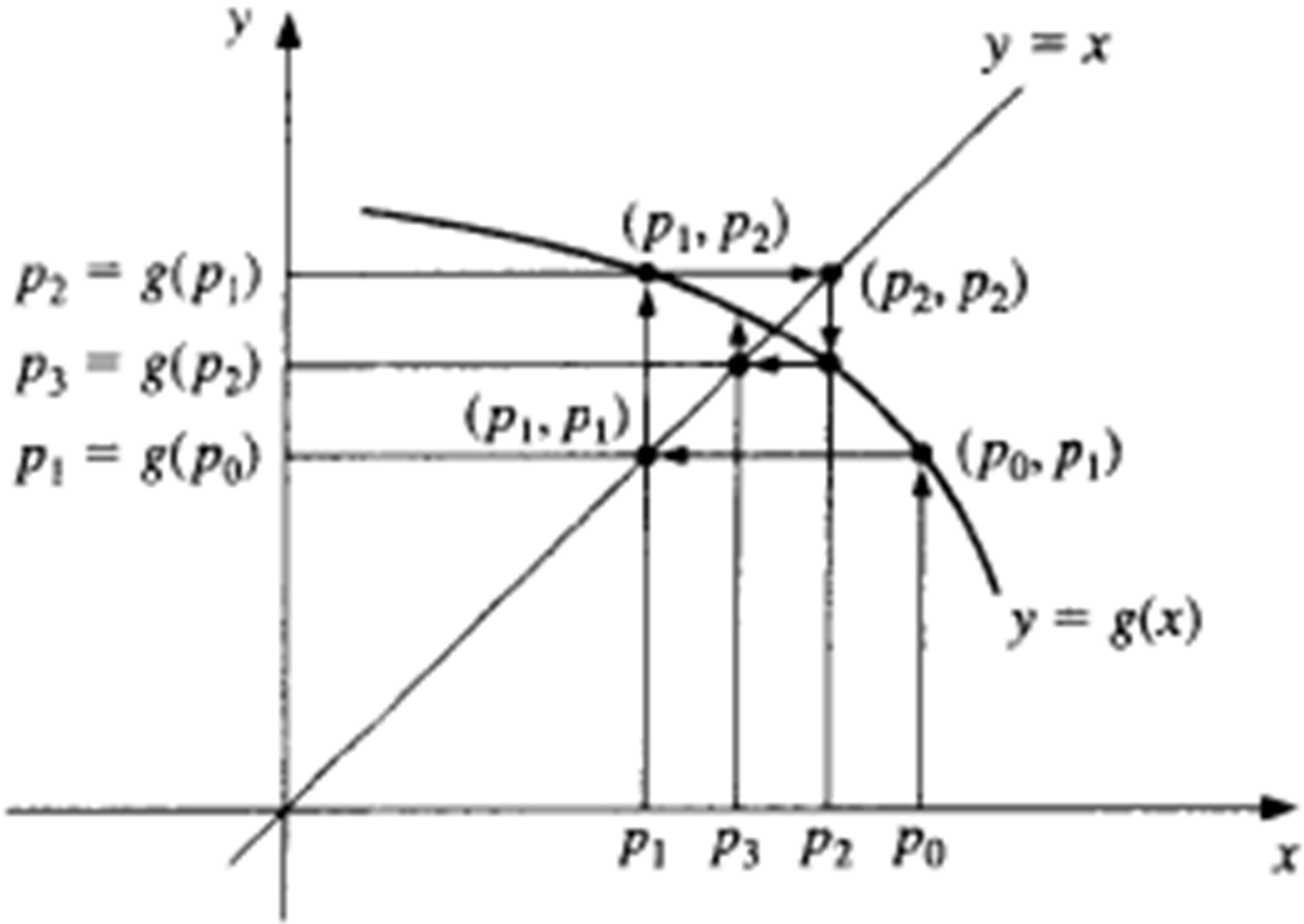
- f(x) = x

$$f(x) + H(x) = g(x) = x - \sin \pi x$$





Fixed Point



Fixed Point

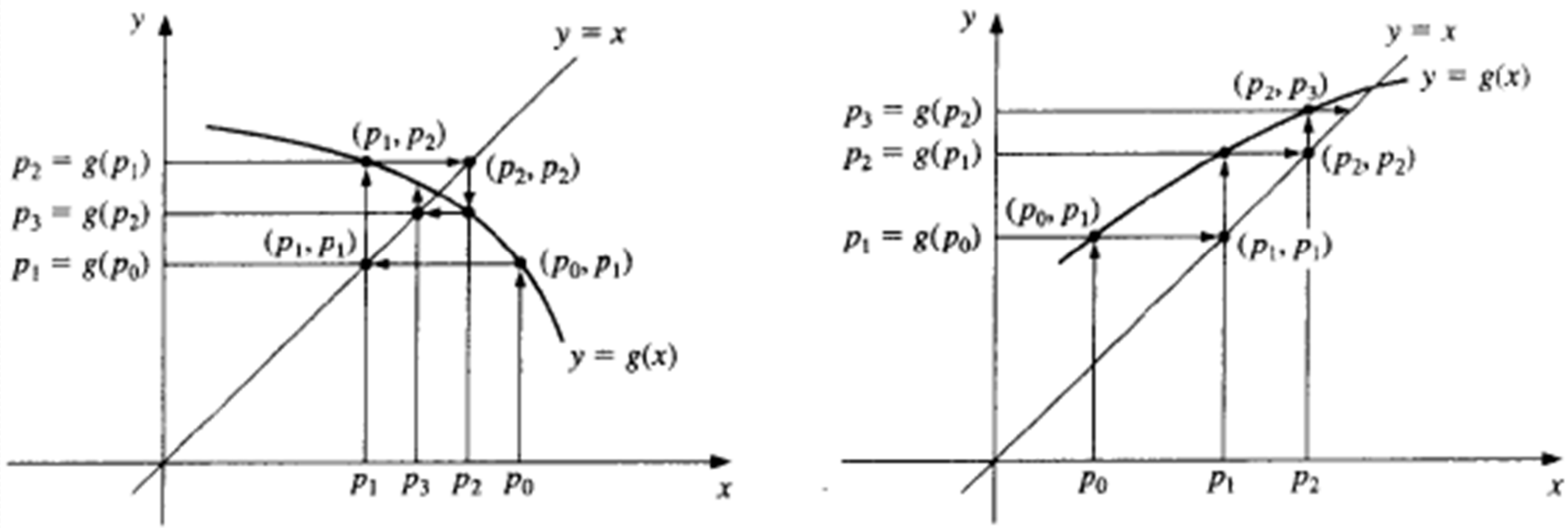
- Pick up a point

- Generate a sequence by letting

$$p_n = g(p_{n-1})$$

- Hopefully you will get the fix point if n is sufficiently large.

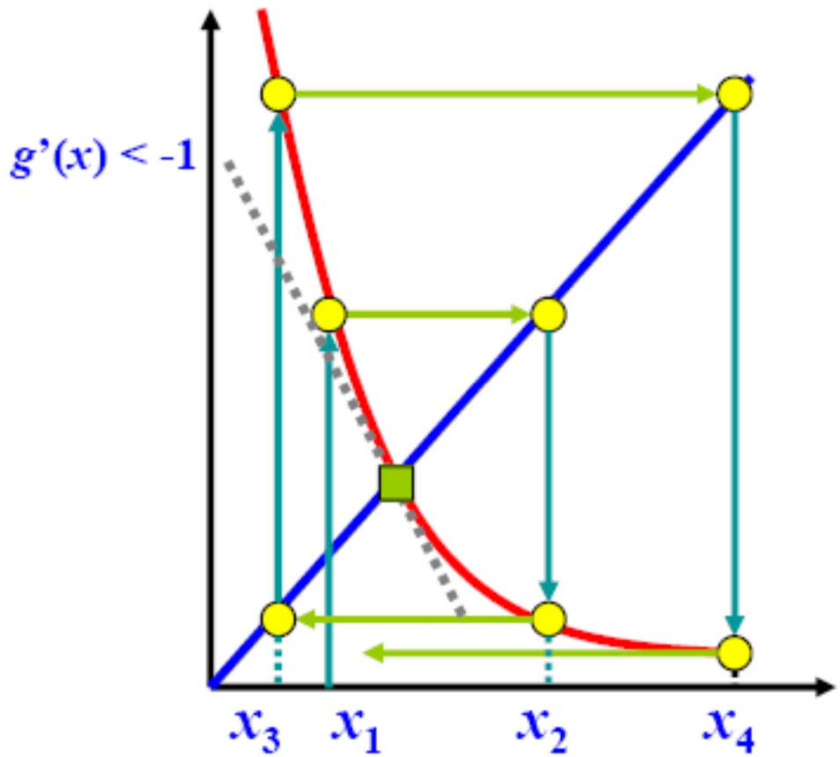
Fixed Point

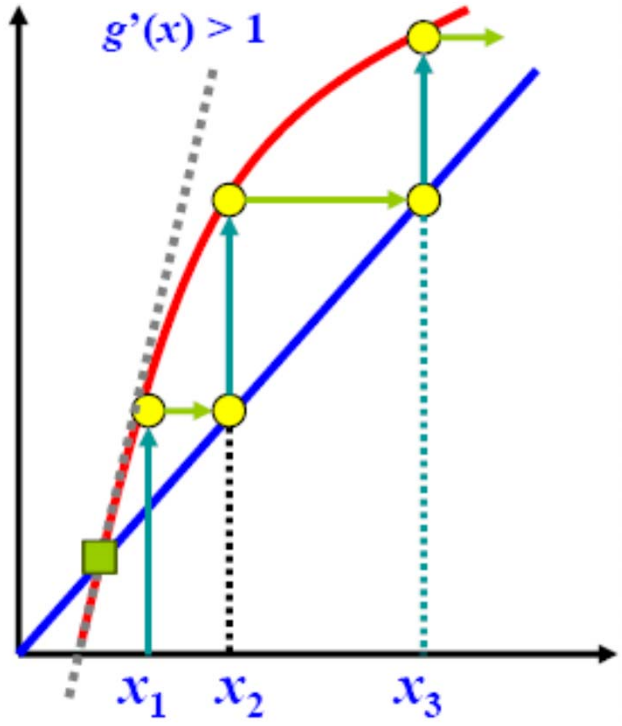


y
y = x
(p_1, p_2)
$p_2 = g(p_1)$
(p_2, p_2)
$p_3 = g(p_2)$
(p_1, p_1)
$p_1 = g(p_0)$
(p_0, p_1)
y = g(x)
p_1
p_3
p_2
p_0
x
y
y = x
y = g(x)
(p_2, p_3)
$p_3 = g(p_2)$
$p_2 = g(p_1)$
(p_2, p_2)
(p_0, p_1)
$p_1 = g(p_0)$
(p_1, p_1)
p_0
p_1
p_2
x

Fixed Point

- Case of divergence





Fixed Point Method

- Convergence is not guaranteed.

It requires careful fixed pt conversion

- It could work faster than multiple partition method
- Shorter code.

Newton Raphson Method

Newton Raphson Method

- Aka. Newton's Method
- Based on linear approximation of Taylor's Expansion

$$f(x) = f(p_0) + f'(p_0)(x - p_0) + \frac{1}{2} f''(p_0)(x - p_0)^2 + \ldots$$

Newton Raphson Method

- If $p \neq p_0$ is a root of f

$$0 = f(p) = f(p_0) + f'(p_0)(p - p_0) + \frac{1}{2} f''(p_0)(p - p_0)^2 + ..$$

- and p_o is pretty close to p

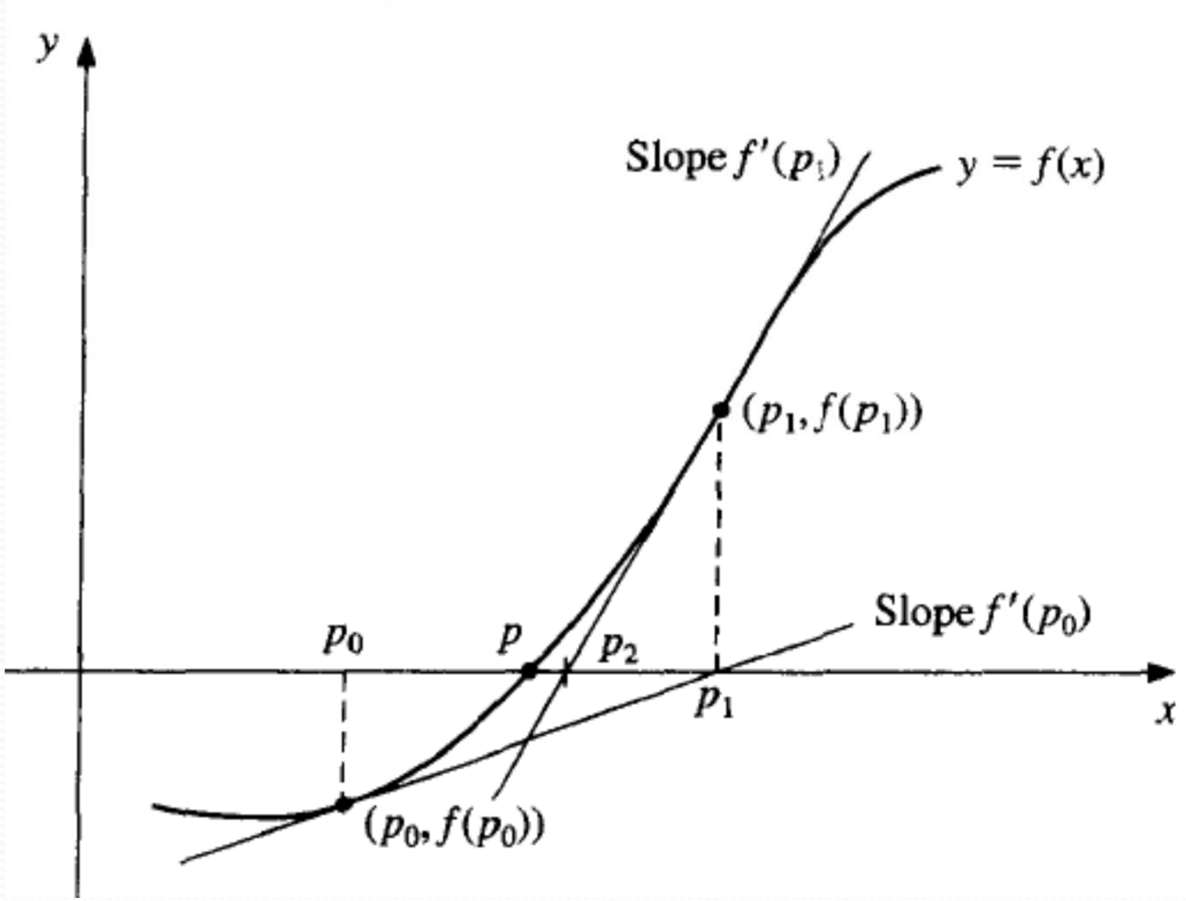
$$p = p_0 - \frac{f(p_0)}{f'(p_0)}$$

Newton Raphson Method

- Selecting an approximation value p_o
- Estimate the function value and the derivative at p_o
- Apply the following equation until the estimation reaches the stop criteria

$$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}$$

Newton Raphson Method



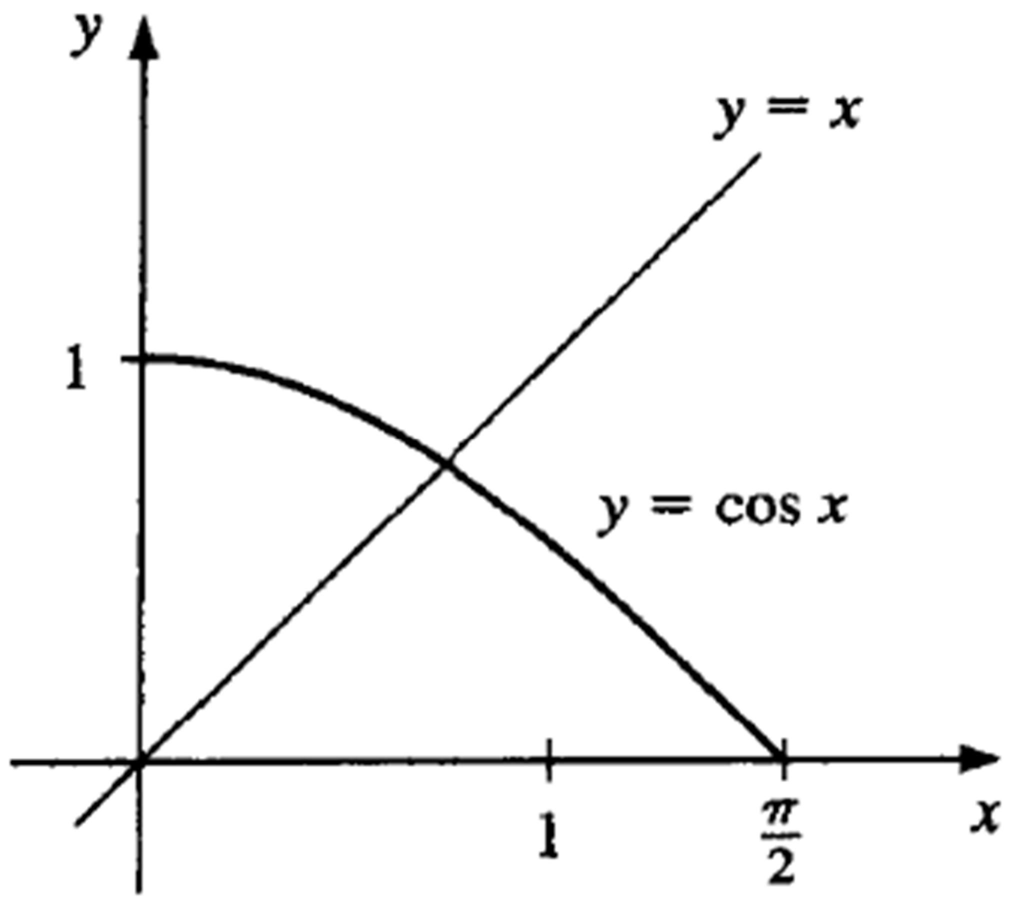
Newton Raphson Method

- When to stop?
- Setting the error tolerance
- Stop when one of these criteria is satisfied.
  - If p is away from 0 $$\frac{|p_N - p_{N-1}|}{|p_N|} < \varepsilon$$
  - If p is close to 0 $$|p_N - p_{N-1}| < \varepsilon$$
  - Directly test the result

$$f(p_N) < \varepsilon$$

Example(I)

- Find a root of x-cos(x)=0;



Example(I)

- Start from $p_o = \frac{\pi}{4}$

$$f(x) = x - \cos x \qquad f'(x) = 1 + \sin x$$

- Calculate p_1 according to Newton's Method

$$f\left(\frac{\pi}{4}\right) = \frac{\pi}{4} - \frac{\sqrt{2}}{2} \qquad f'\left(\frac{\pi}{4}\right) = 1 + \frac{\sqrt{2}}{2}$$

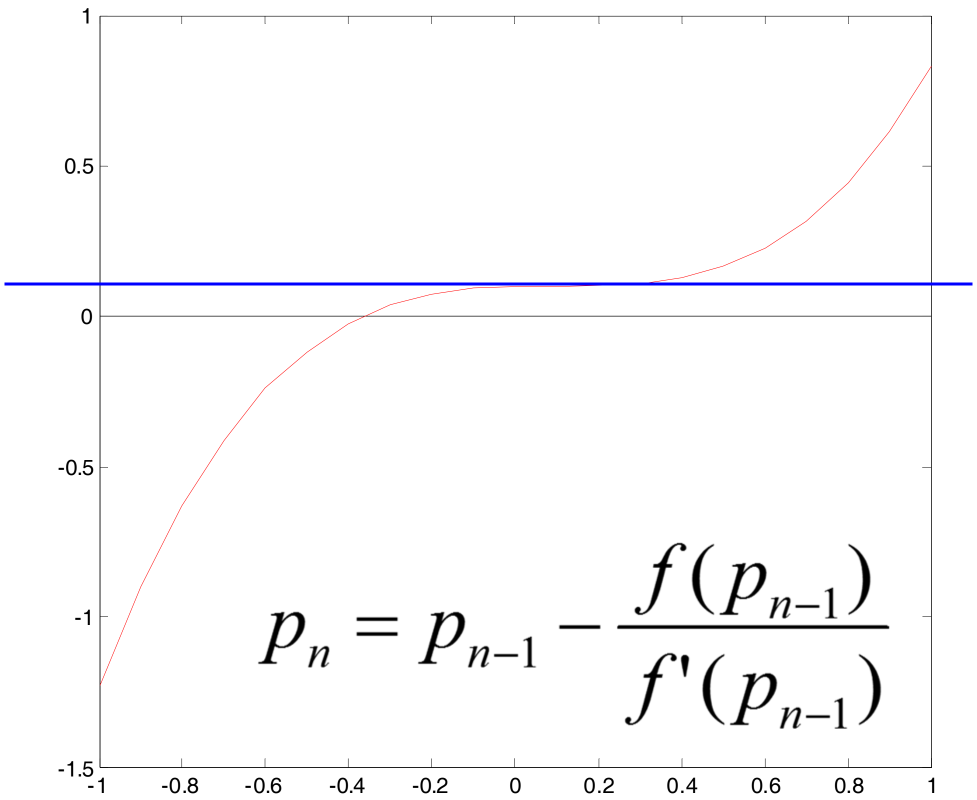
$$p_1 = \frac{\pi}{4} - \frac{\frac{\pi}{4} - \frac{\sqrt{2}}{2}}{1 + \frac{\sqrt{2}}{2}} = 0.73954$$

Example(I)

n	p	f(p)	f'(p)
0	0.785398163	0.078291	1.707107
1	0.739536134	0.000755	1.673945
2	0.739085178	7.51E-08	1.673612
3	0.739085133	0	1.673612
4	0.739085133	0	1.673612
5	0.739085133	0	1.673612

Weakness of Newton's Method

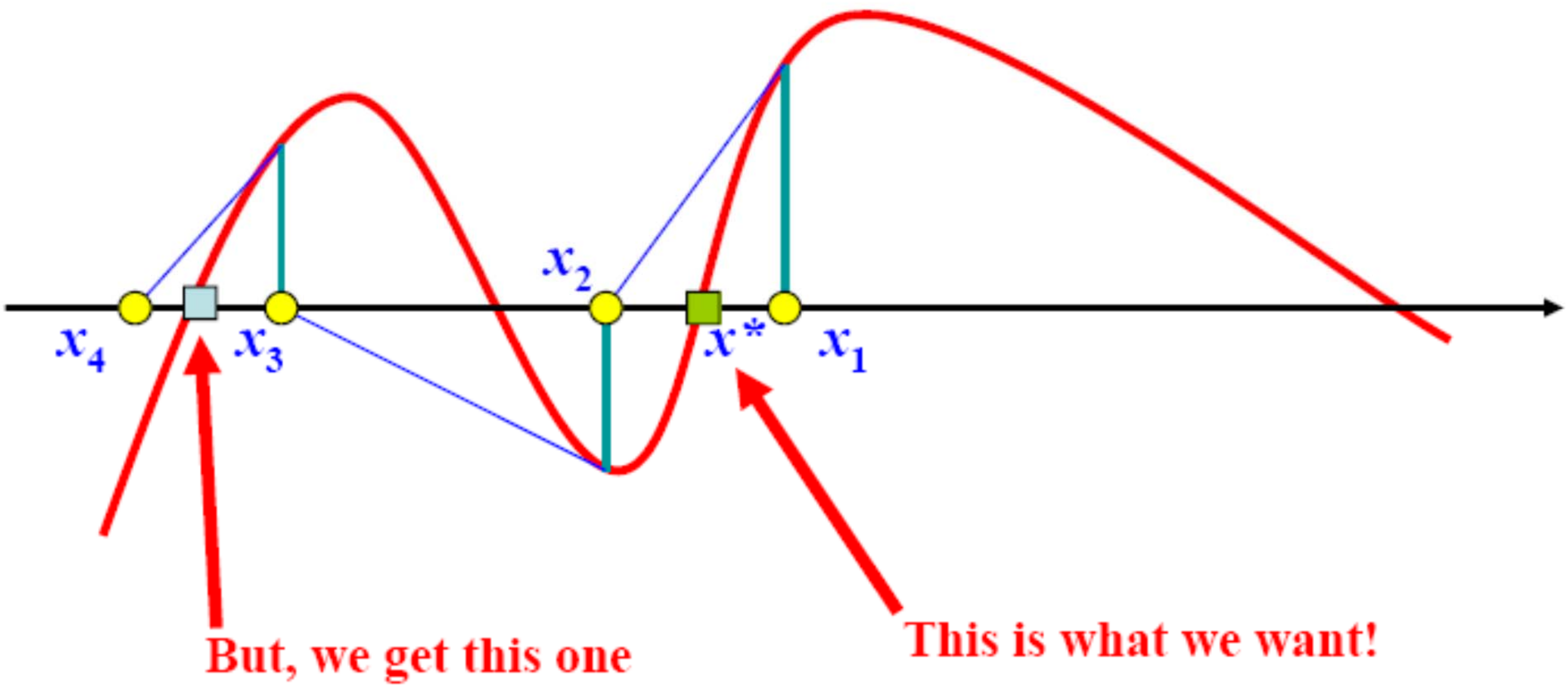
- Zero Slope



$$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}$$

Weakness of Newton's Method

- Converge to other roots



Weakness of Newton's Method

- Solve the equation using Newton's Method

$$f(x) = x^3 - 3x^2 + x + 3 = 0$$

- The derivative is

$$f'(x) = 3x^2 - 6x + 1$$

- The iteration process

$$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}$$

Weakness of Newton's Method

- Start from $p_0 = 1$

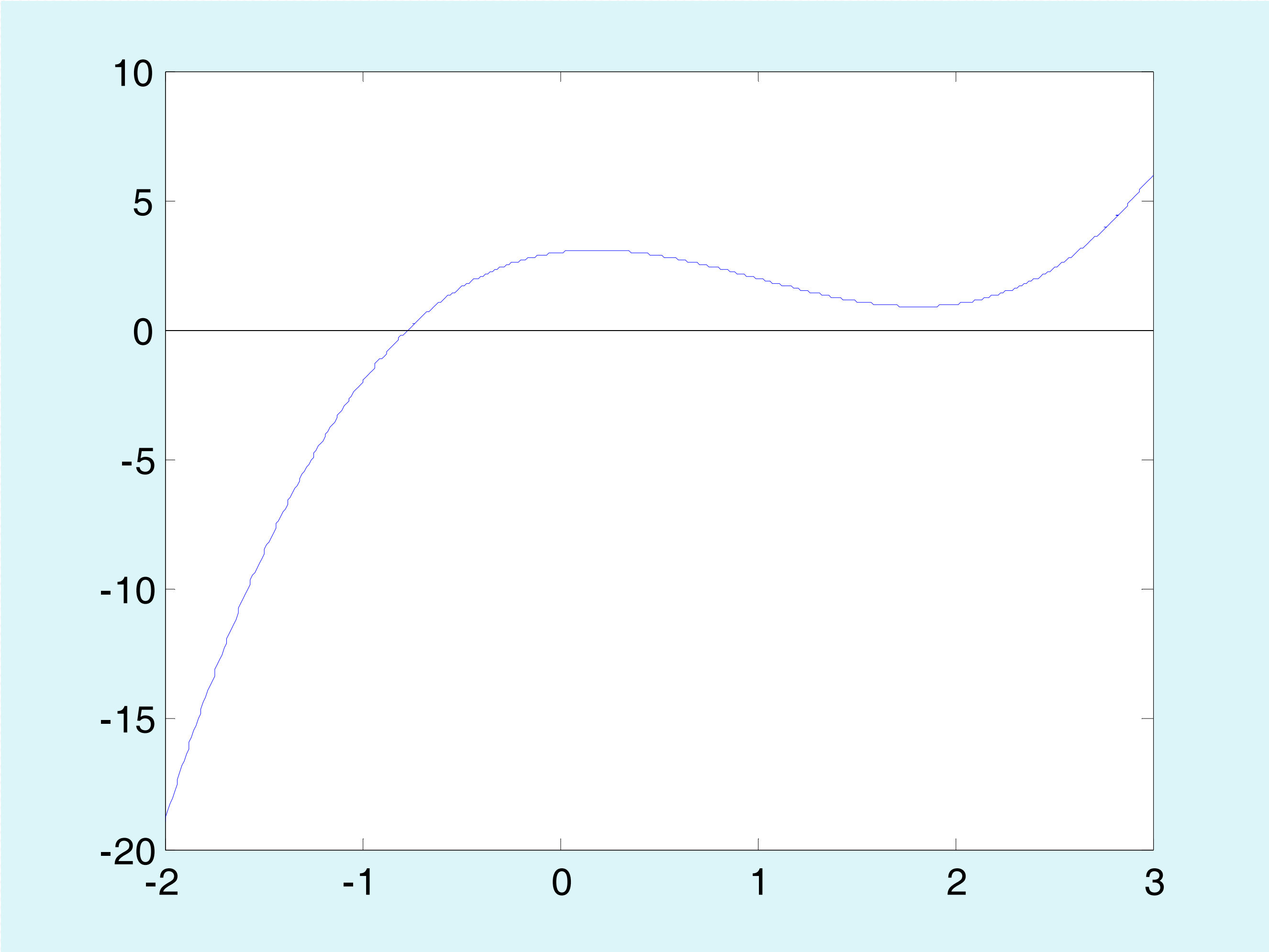
$$p_1 = 1 - \frac{f(1)}{f'(1)}$$

$$p_1 = 1 - \frac{2}{-2} = 2$$

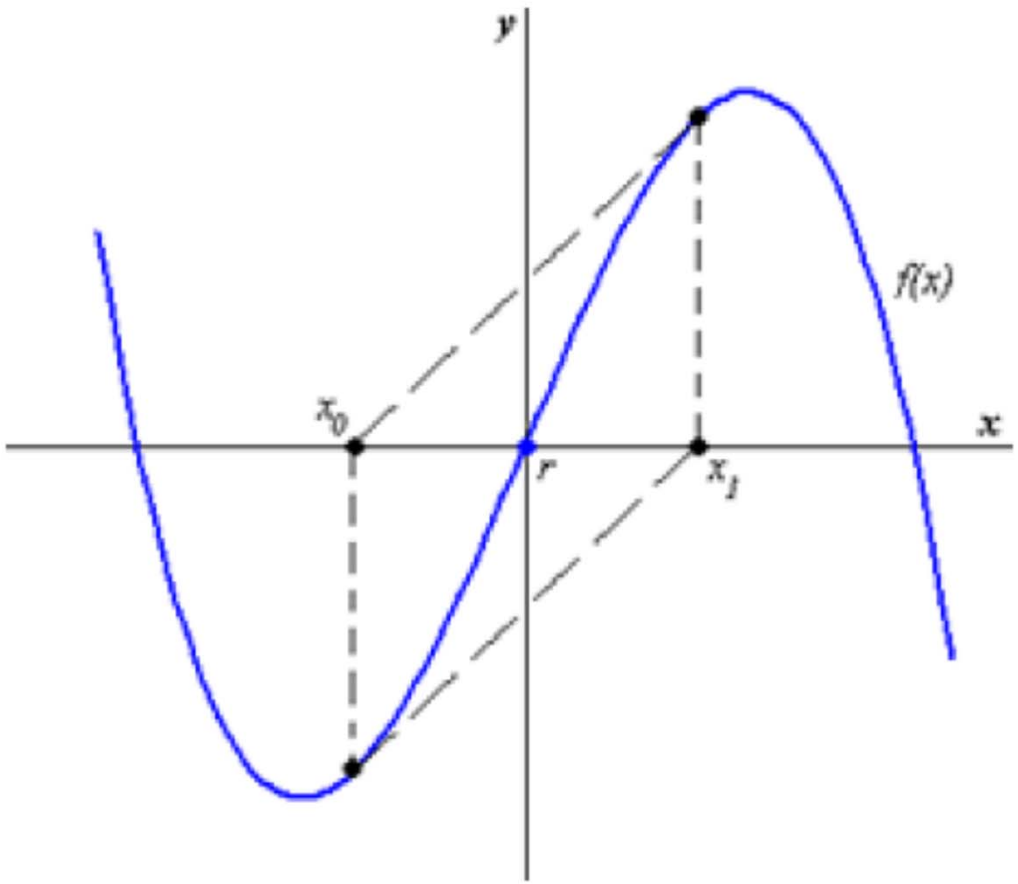
$$p_2 = 2 - \frac{1}{1} = 1$$

n	p	f(p)	f'(p)
0	1	2	-2
1	2	1	1
2	1	2	-2
3	2	1	1
4	1	2	-2
5	2	1	1

Weakness of Newton's Method

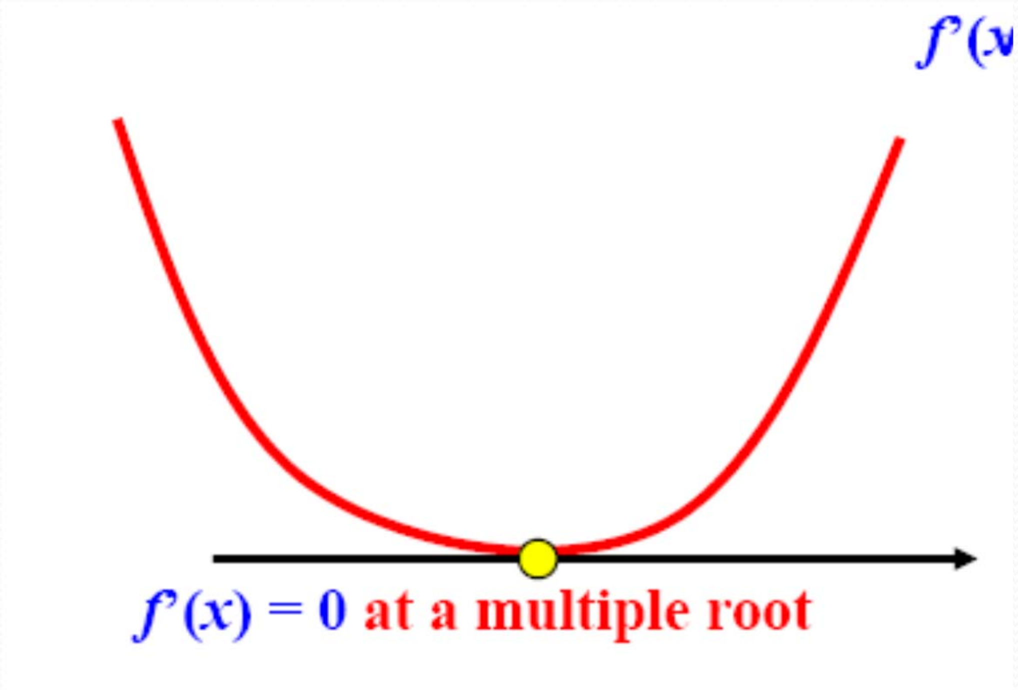


Weakness of Newton’s Method



Weakness of Newton's Method

- When a root of multiplicity exists



Example(II)

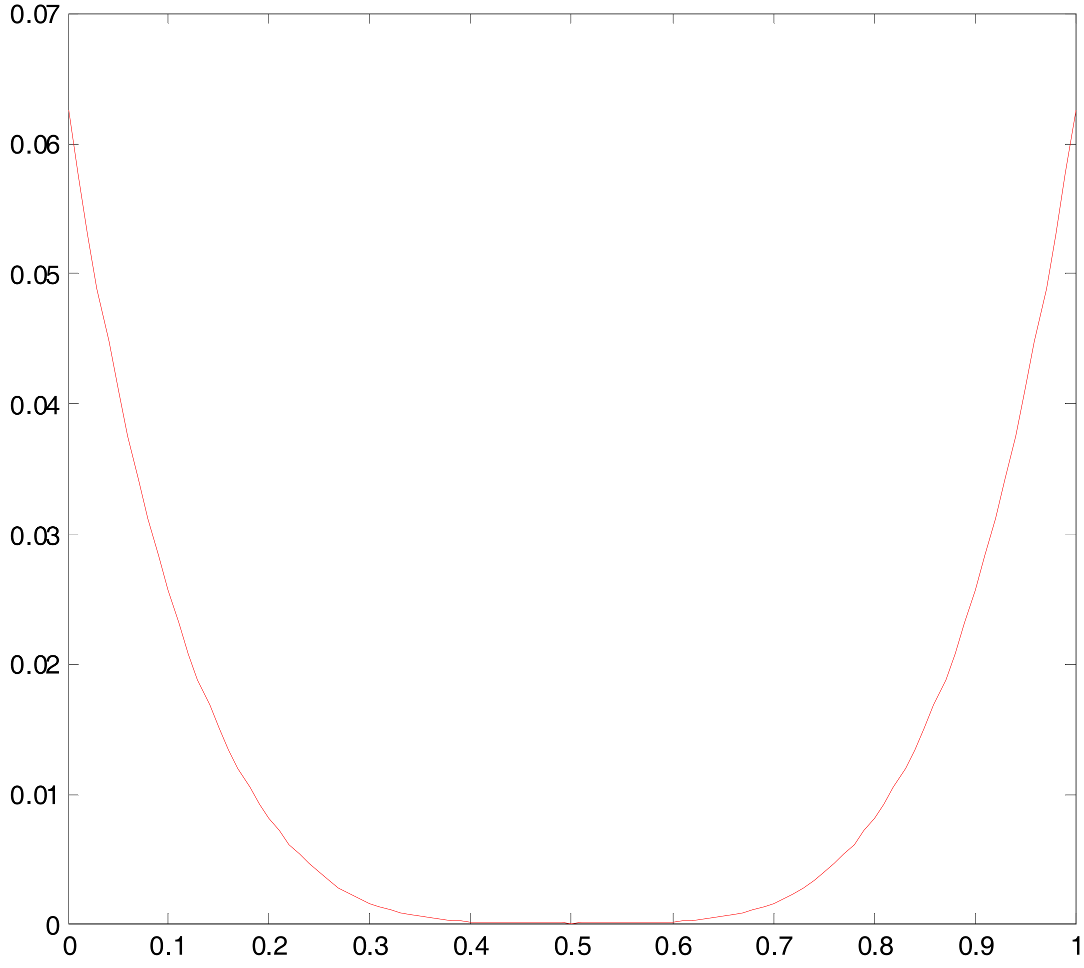
- Use Newton's Method to find the root of the equation

$$f(x) = (x-0.5)^4 = 0$$

- The derivative

$$f'(x) = 4(x-0.5)^3$$

Example(II)



Example(II)

n	p	f(p)	f′(p)
0	1	0.0625	0.5
1	0.875	0.019775	0.210938
2	0.78125	0.006257	0.088989
3	0.7109375	0.00198	0.037542
4	0.658203125	0.000626	0.015838
5	0.618652344	0.000198	0.006682
6	0.588989258	6.27E-05	0.002819
7	0.566741943	1.98E-05	0.001189
8	0.550056458	6.28E-06	0.000502
9	0.537542343	1.99E-06	0.000212
10	0.528156757	6.29E-07	8.93E-05
11	0.521117568	1.99E-07	3.77E-05
12	0.515838176	6.29E-08	1.59E-05

n	p	f(p)	f′(p)
0	0.51	1E-08	4E-06
1	0.5075	3.16E-09	1.69E-06
2	0.505625	1E-09	7.12E-07
3	0.50421875	3.17E-10	3E-07
4	0.503164063	1E-10	1.27E-07
5	0.502373047	3.17E-11	5.35E-08
6	0.501779785	1E-11	2.26E-08
7	0.501334839	3.17E-12	9.51E-09
8	0.501001129	1E-12	4.01E-09
9	0.500750847	3.18E-13	1.69E-09
10	0.500563135	1.01E-13	7.14E-10
11	0.500422351	3.18E-14	3.01E-10
12	0.500316764	1.01E-14	1.27E-10

Example(II)

- The convergence of Newton's Method at a root of multiplicity will be pretty slow

- The slope is almost 0 in the neighborhood of the root, leading to slow convergence.

- In case of root of multiplicity, Newton's method shall be remodeled

Reminder

- If f(x) has a root of multiplicity of m at p
- then $f(p)=f'(p)=\ldots=f^{(m-1)}(p)=0$; and $f^{(m)}(p)\neq 0$
- Ex:

$$f(x)=(x-0.5)^4 \qquad f'(x)=4(x-0.5)^3$$

$$f''(x)=12(x-0.5)^2 \qquad f'''(x)=24(x-0.5)$$

Modified Newton Raphson Method

- The iteration of Newton's Method

$$p_{n+1} = p_n - \frac{f(p_n)}{f'(p_n)}$$

- Define a new function

$$\mu(x) = \frac{f(x)}{f'(x)}$$

- And p is also a root of

$$\mu(p) = \frac{f(p)}{f'(p)} = 0$$

Newton Raphson Method

- Take a look at μ(x)
- Suppose f(x) has a root at p of multiplicity of m; f'(x) will have p as a root of multiplicity of (m-1)

$$f(x)=(x-p)^m q(x) \quad \text{and} \quad f'(x)=(x-p)^{m-1}[mq(x)+(x-p)q'(x)]$$

- Then

$$\mu(x)=\frac{f(x)}{f'(x)}=\frac{(x-p)^m q(x)}{m(x-p)^{m-1}q(x)+(x-p)^m q'(x)}=\frac{(x-p)q(x)}{mq(x)+(x-p)q'(x)}$$

- μ(x) has only simple zero at p

Modified Newton Raphson Method

- The iteration becomes

$$p_{n+1} = p_n - \frac{\mu(p_n)}{\mu'(p_n)}$$

- or

$$p_{n+1} = p_n - \frac{\mu(p_n)}{\mu'(p_n)} = p_n - \frac{f(p_n)f'(p_n)}{f'(p_n)^2 - f(p_n)f''(p_n)}$$

Example(III)

- Use Modified Newton Raphson Method to find a root of the equation

$$f(x) = (x-0.5)^4 = 0$$

- The derivatives are

$$f'(x) = 4(x-0.5)^3$$

$$f''(x) = 12(x-0.5)^2$$

Example(III)

- Start From po = 2

$$f(2) = (2-0.5)^4$$

$$f'(2) = 4(2-0.5)^3$$

$$f''(2) = 12(2-0.5)^2$$

$$p_1 = p_0 - \frac{4(2-0.5)^3(2-0.5)^4}{[4(2-0.5)^3]^2 - 12(2-0.5)^2(2-0.5)^4}$$

$$= (2-0.5)$$

$$p_1 = 1.5$$

- Start From po = 0.51

$$p_0 = 0.51$$

$$p_1 = 0.51 - 0.01$$

Example(III-b)

- Use Modified Newton Raphson Method to find a root of the equation

$$f(x) = e^x - x - 1 = 0$$

- The derivatives are

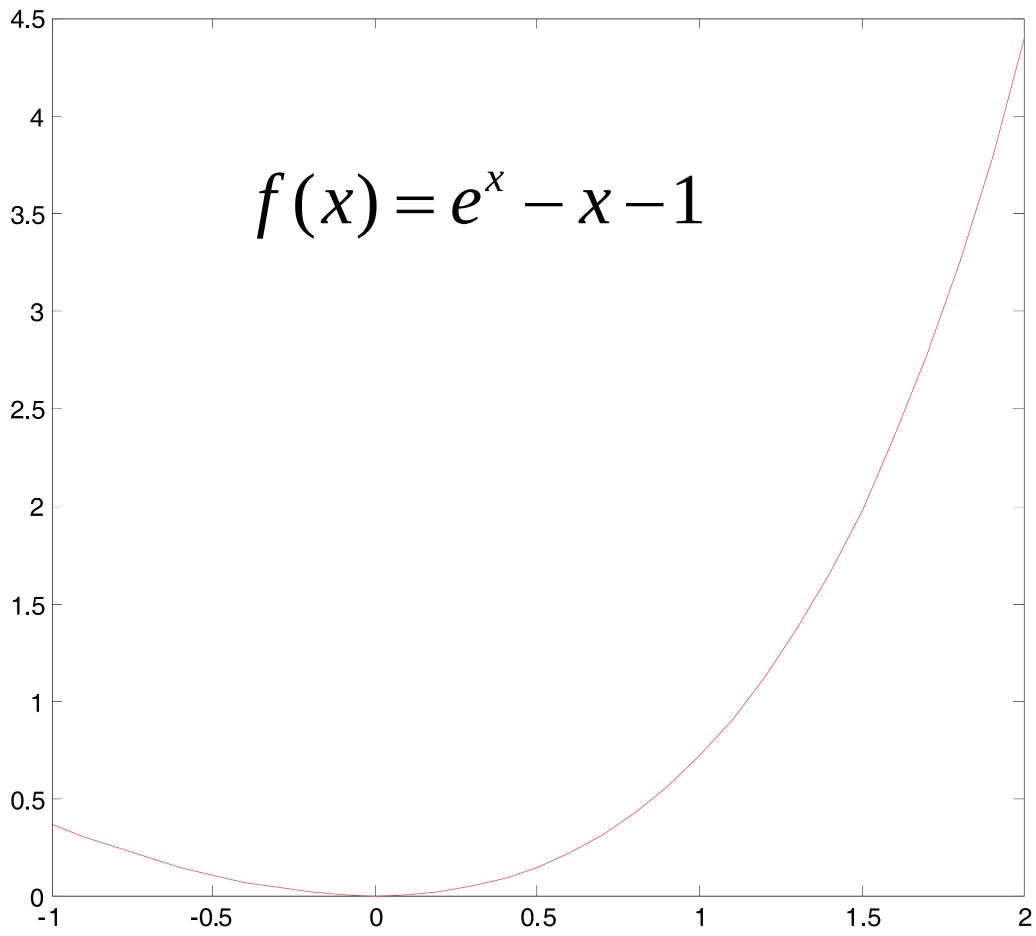
$$f'(x) = e^x - 1$$

$$f''(x) = e^x$$

Example(III-b)

n	Newton	M_newton	f(p)	f'(p)	f(p)	f'(p)	f''(p)
0	1	1	0.718282	1.718282	0.718282	1.718282	2.718282
1	0.581977	-0.23421	0.207596	0.789572	0.025406	-0.2088	0.791195
2	0.319055	-0.00846	0.056772	0.375827	3.57E-05	-0.00842	0.991577
3	0.167996	-1.2E-05	0.014936	0.182932	7.07E-11	-1.2E-05	0.999988
4	0.086349	-4.2E-11	0.003838	0.090187	0	-4.2E-11	1
5	0.043796	-4.2E-11	0.000973	0.044769	0	-4.2E-11	1

Example(III-b)



Example(IV)

- Compare the Newton's Method and modified Newton Raphson Method to solve

$$f(x) = x - \cos x = 0$$

- Comparison of the two methods

n	Newton	M_newton
0	1	1
1	0.750363868	0.730634099
2	0.739112891	0.739069143
3	0.739085133	0.739085133
4	0.739085133	0.739085133
5	0.739085133	0.739085133

Modified Newton Raphson Method

- Higher order derivative and additional calculation are required
- Convert the original function that has a root of multiplicity to a simple zero function.
- Accelerate convergence for root of multiplicity
- If the original problem has only simple zero, it is still applicable but has no effect on convergence.

Newton Raphson Method

- What about complex roots

$$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}$$

- If coefficients of f(x) are all real, and initial guess of p is also real, the algorithm will fail to find a complex root

- Initial guess is allowed to be complex.

Example(V)

- Find a root of the equation

$$f(x) = x^2 + 2x + 5$$

- The derivative is

$$f'(x) = 2x + 2x$$

- Iteration process

$$p_n = p_{n-1} - \frac{f(x)}{f'(x)}$$

Example(V)

n	p	p^2+2p+5	2p+2
0	1.5	10.25	5
1	-0.55	4.2025	0.9
2	-5.21944	21.80371	-8.43889
3	-2.63573	6.6756	-3.27145
4	-0.59516	4.163892	0.809671
5	-5.73786	26.44733	-9.47572
6	-2.9468	7.790027	-3.8936
7	-0.94607	4.002908	0.107856
8	-38.0597	1377.418	-74.1193

n	p	p^2+2p+5	2p+2
0	1 + 1i	7 + 4i	4 + 2i
1	-0.8 + 0.9i	3.23 + 0.36i	0.4 + 1.8i
2	-1.3706 + 2.5676i	-2.4555 - 1.9031i	-0.7412 + 5.1353i
3	-1.0752 + 2.0469i	-0.184 - 0.3077i	-0.1503 + 4.0937i
4	-1.0017 + 1.9992i	0.0031 - 0.007i	-0.0035 + 3.9984i
5	-1 + 2i	0 + 0i	0 + 4i

Newton Raphson Method

- Fast convergence is the initial guess is appropriate.
- A prototype for several root finding or optimization problem
- When multiple roots are present, use modified Newton Raphson Method.

Newton Raphson Method

- Weakness of Newton's Method can be avoided by carefully choosing the initial guess
  - Local Minimum
  - Inflection Point

- Typically Multiple partition will be first use to find the neighborhood of a root, then apply Newton's Method to refine the root.

- Newton Raphson's Method is compatible to locate complex roots.
  - A complex initial guess must be taken

Secant Method

- Newton's Method

$$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}$$

- What if you have this problem?

$$f(x) = x^2 e^{-x} \sin(x)$$

$$f'(x) = 2xe^{-x}\sin(x) - x^2 e^{-x}\sin(x) + x^2 e^{-x}\cos(x)$$

Secant Method

- Approximation of derivative

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

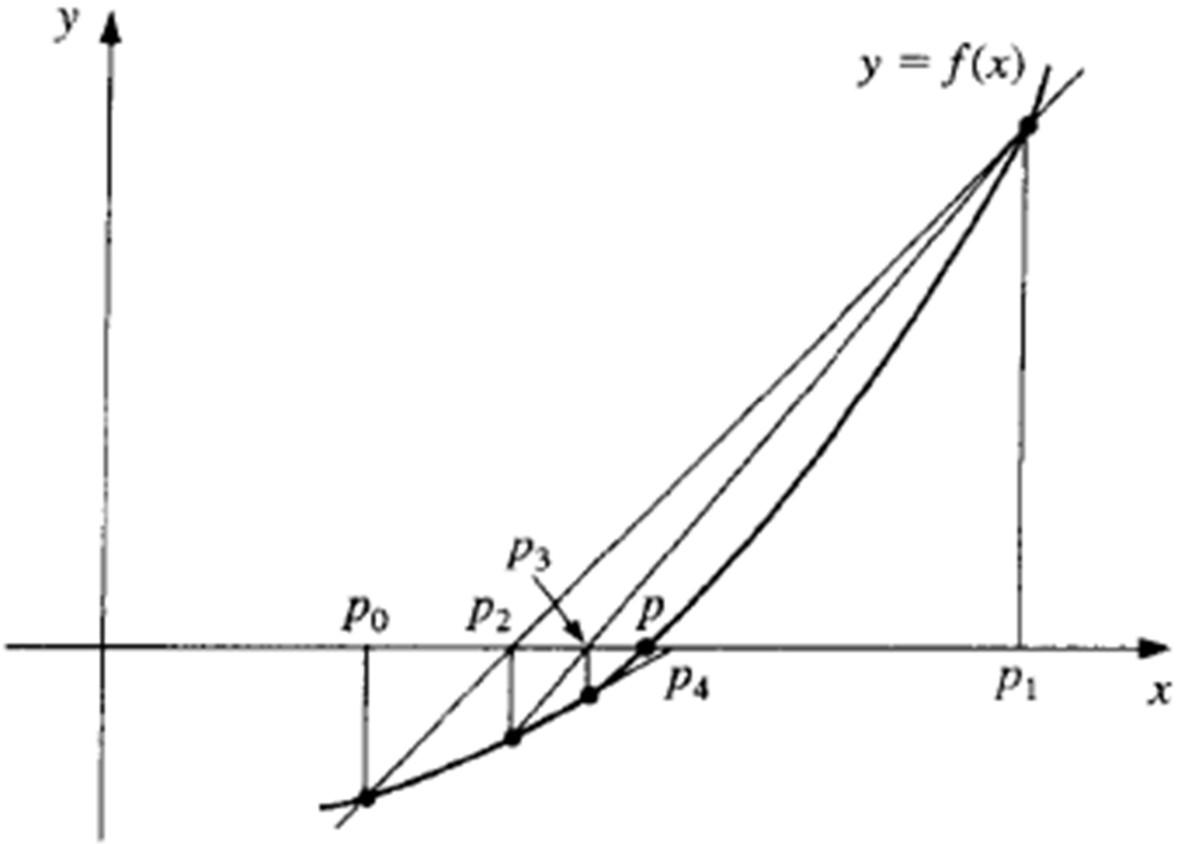
- When it comes to root finding

$$f'(p_n) \approx \frac{f(p_n) - f(p_{n-1})}{p_n - p_{n-1}}$$

Secant Method

- Selecting two initial points x_0 and x_1
- Find the x intercept of the secant line. Now the new point is x_2
- Evaluate corresponding $f(x_2)$
- Use x1 and x_2 to find a new intercept as x_3
- Apply the following equation until the estimation reaches the stop criteria

Secant Method



Secant Method

- The iterative relation of the approximated roots
- Newton's Method
- Secant Approximation $$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}$$
- Secant Method $$f'(p_{n-1}) \approx \frac{f(p_{n-1}) - f(p_{n-2})}{p_{n-1} - p_{n-2}}$$

$$p_n = p_{n-1} - \frac{f(p_{n-1})(p_{n-1} - p_{n-2})}{f(p_{n-1}) - f(p_{n-2})}$$

Example

- Find a zero of

$$f(x) = x - \cos x$$

- Two initial points are needed.
  - $P_0 = 0.5$ $p_1 = \dfrac{\pi}{4}$

$$p_n = p_{n-1} - \frac{(p_{n-1} - \cos p_{n-1})(p_{n-1} - p_{n-2})}{(p_{n-1} - \cos p_{n-1}) - (p_{n-2} - \cos p_{n-2})}$$

Example

n	p	p-cos(p)
0	0.5	-0.377583
1	0.7853982	0.0782914
2	0.7363841	-0.004518
3	0.7390581	-4.52E-05
4	0.7390851	2.698E-08
5	0.7390851	-1.61E-13
6	0.7390851	0

Example

Secant Method

n	p	p-cos(p)
0	0.5	-0.377583
1	0.7853982	0.0782914
2	0.7363841	-0.004518
3	0.7390581	-4.52E-05
4	0.7390851	2.698E-08
5	0.7390851	-1.61E-13
6	0.7390851	0

Newton Raphson Method

n	p	f(p)	f'(p)
0	0.785398163	0.078291	1.707107
1	0.739536134	0.000755	1.673945
2	0.739085178	7.51E-08	1.673612
3	0.739085133	0	1.673612
4	0.739085133	0	1.673612
5	0.739085133	0	1.673612

Secant Method

- Secant Method reduces computation of complex derivative
- The convergence is a little bit slower to Newton's Method
- Sometimes the approximated root will go out of the two end points

Brief Summary of Newton Raphson Method

- Linear approximation is the fundamental of Newton's Method
- Initial guess and the behavior of the function is critical to convergence of the algorithm
- Newton's Method using tangent line requires calculation of derivatives which may take much more additional computation
- Secant Method has slightly slower rate of convergence than Tangent Method. But in some occasion, it saves time in functional evaluation.