Chap 1: Solving Nonlinear Eq.

- Interval Halving (Bisection)
- Linear Interpolation Methods
- Newton's Method
- Muller's Method
- Fixed-Point Iteration
- Order of convergence
- Multiple Roots
- Nonlinear systems

Introduction -1

- **Problem: Solve f(x)=0**
  - **A system of nonlinear equations**

$$f_1(x_1, x_2, \ldots\ldots, x_n) = 0$$
$$\vdots$$
$$f_n(x_1, x_2, \ldots\ldots, x_n) = 0$$

- **Nonlinear function can be**
  - **Polynomials**

$$f(x, y) = \sum_{i+j=n} a_{ij} x^i y^j$$

  - **Functions involve transcendental functions**
    - **sin, cos, exponentials**

Introduction -2

- Closed form solutions
  - Only available for polynomials of degree less than 5.
    - Quadratic formula for degree 2
    - Complicated for degrees 3 and 4
  - For nonlinear polynomial system
    - Algebraic methods such as Grobner basis can be applied to eliminate variables and reduce the system to a triangular form

Introduction -3

- **Numerical solutions**
  - **Via iteration procedure**
    - **Starting point**
    - **Compute iterates**
    - **Check for termination**
  - **Need to consider**
    - **Convergence**
    - **Rate of convergence**
    - **Stability**
      - **Early error magnified or not?**

Bisection method -1

- An ancient but effective method for solving $f(x)=0$
- Starting with $[x_1, x_2]$: an interval that bracket a root, with $f(x_1)*f(x_2) < 0$
  - f changes signs at x_1 and x_2
  - If f is continuous, there must be at least one root between x_1 and x_2
- Divides the interval in half, finds in which half the root must lie, and repeat

Bisection method -2

- **Pseudo code**

$$
\begin{aligned}
&\text{Repeat} \\
&\qquad x_3 = (x_1 + x_2)/2 \\
&\qquad \text{if } \; f(x_3)\,f(x_1) < 0 \\
&\qquad\qquad x_2 = x_3 \\
&\qquad\qquad \text{else } x_1 = x_3 \\
&\text{Until } \left(\left|x_1 - x_2\right|/2 < \text{tolerance}\right)
\end{aligned}
$$

- **The final value of x_3 approximates the root, with error no more than $|x_1-x_2|/2$**
- **The method may produce a false root if f(x) is discontinuous on $[x_1, x_2]$**

Bisection Method -3

- **Advantages**
  - It is guaranteed to work if f(x) is continuous in the initial interval, and if the interval actually brackets a root
  - The number of iterations to achieve a specified accuracy is known in advance, since the interval [a, b] is halved each time, so

$$\text{error after n iterations} < \left|\frac{b-a}{2^n}\right|$$

$$\left|\frac{b-a}{2^n}\right| < \text{Tolerance} \Rightarrow \text{a bound on } n$$

- **Disadvantages**
  - Slow to converge
    - **Why? No information about f(x) is used**

Bisection Method -4

- **An example, a=0, b=1, tolerance=1E-4**

$$f(x) = 3x + \sin(x) - e^{x} = 0$$

Table 1.1 The bisection method for $f(x) = 3x + \sin(x) - e^x = 0$, starting from $x_1 = 0$, $x_2 = 1$, using a tolerance value of 1E-4

Iteration	X_1	X_2	X_3	$F(X_3)$	Maximum error	Actual error
1	0.00000	1.00000	0.50000	0.33070	0.50000	0.13958
2	0.00000	0.50000	0.25000	−0.28662	0.25000	−0.11042
3	0.25000	0.50000	0.37500	0.03628	0.12500	0.01458
4	0.25000	0.37500	0.31250	−0.12190	0.06250	−0.04792
5	0.31250	0.37500	0.34375	−0.04196	0.03125	−0.01667
6	0.34375	0.37500	0.35938	−0.00262	0.01563	−0.00105
7	0.35938	0.37500	0.36719	0.01689	0.00781	0.00677
8	0.35938	0.36719	0.36328	0.00715	0.00391	0.00286
9	0.35938	0.36328	0.36133	0.00227	0.00195	0.00091
10	0.35938	0.36133	0.36035	−0.00018	0.00098	−0.00007
11	0.36035	0.36133	0.36084	0.00105	0.00049	0.00042
12	0.36035	0.36084	0.36060	0.00044	0.00024	0.00017
13	0.36035	0.36060	0.36047	0.00013	0.00012	0.00005

Bisection Method -5

- Some comments
  - Recommended: used for finding an approximate value for the root, and the value is refined by more efficient methods
    - Most other root-finding methods require a starting value near to a root – lacking this, they may fail completely
    - Good practice:
      - Graph the function first
      - Search for interval that with sign change at ends
      - Apply Bisection to get an initial starting value
      - Apply better methods
  - Not applicable to the case of multiple roots
    - Find the root by working on with f'(x), which will be zero at a multiple root.

Linear Interpolation Methods

- **Approximate the function by a straight line**
  - **Interpolated line**
    - **The secant method**
      - **Two x-values nearest to the root**
    - **False position method**
      - **Similar to the Bisection method**
      - **Two points need to bracket the root**
  - **Tangent line**
    - **Newton method**

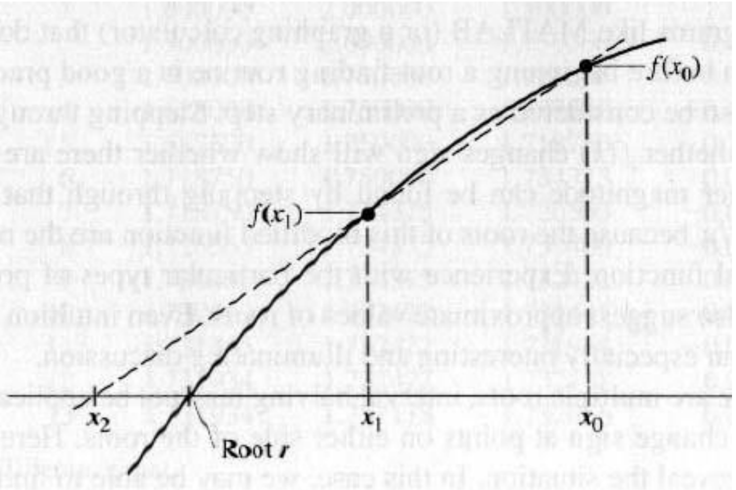


Figure 1.1

Secant method -1

- **Secant method**
  - Find two points on the curve near to the root
    - Draw a graph or apply a few iteration of bisection.
    - Two point may both be on one side of the root, or on opposite sides
  - Find the line through these two points and find the point it intersects the x-axis
  - Repeat the process until the intersection point is close enough to the root.

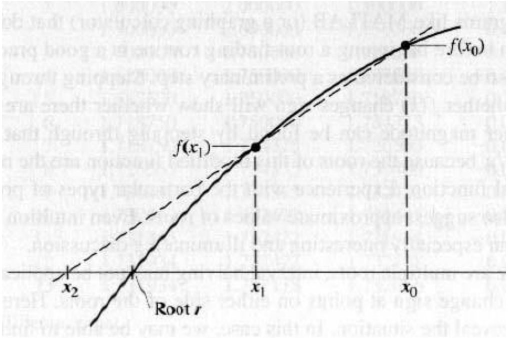


Figure 1.1

Secant method -2

From the similar triangles, we have

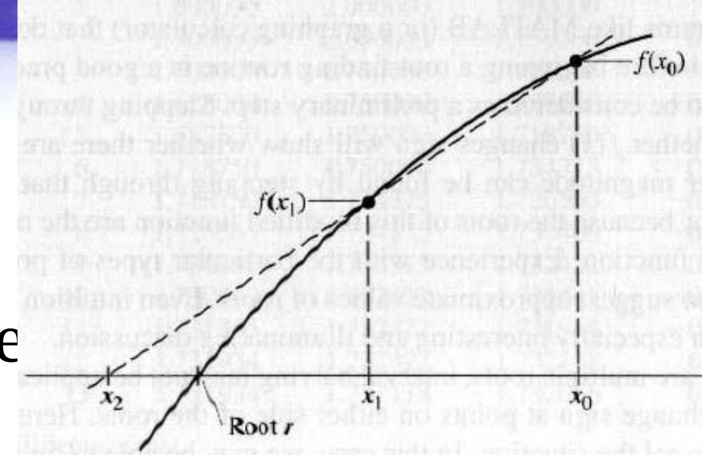
$$\frac{(x_1 - x_2)}{f(x_1)} = \frac{(x_0 - x_1)}{f(x_0) - f(x_1)}$$

Solve for x_2 :

$$x_2 = x_1 - f(x_1)\frac{(x_0 - x_1)}{f(x_0) - f(x_1)}$$

Repeat the iteration, we have

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



Each newly computed value should be nearer to the root.

After second iteration:
Always using the last two computed values.

After first iteration:
There aren't two last computed values.
Swap x0 and x1 if Necessary, such that x1 is closer to the root.

The Secant Method -3

- **Start with x_0 and x_1 near the root**

if $|f(x_0)| < |f(x_1)|$ then swap x_0 and x_1

Repeat

$$x_2 = x_1 - \frac{f(x_1)(x_0 - x_1)}{f(x_0) - f(x_1)}$$

$$x_0 = x_1$$

$$x_1 = x_2$$

Until $|f(x_2)| <$ tolerance value

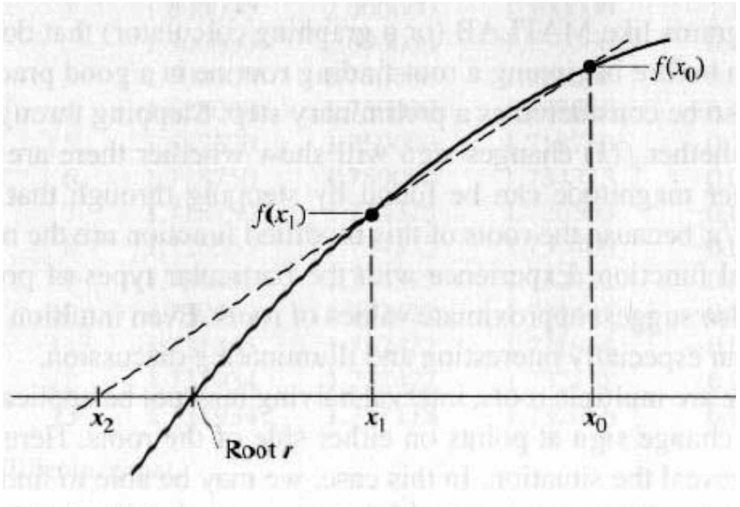


Figure 1.1

Note:

If f(x) is not continuous, the method may fail.

The Secant Method -4
An Example

Table 1.2 Secant method on $f(x) = 3x + \sin(x) - e^x$

Iteration	x_0	x_1	x_2	$f(x_2)$
1	1	0	0.4709896	0.2651588
2	0	0.4709896	0.3722771	2.953367E-02
3	0.4709896	0.3722771	0.3599043	−1.294787E-03
4	0.3722771	0.3599043	0.3604239	5.552969E-06
5	0.3599043	0.3604239	0.3604217	3.554221E-08

At x = .3604217, tolerance of .0000001 met!

- **Fewer iterations are required compared to bisection: 5 iterations**

The Secant Method -5 Problems

- **If the function is far from linear near the root, the successive iterates can fly off to points far from the root**

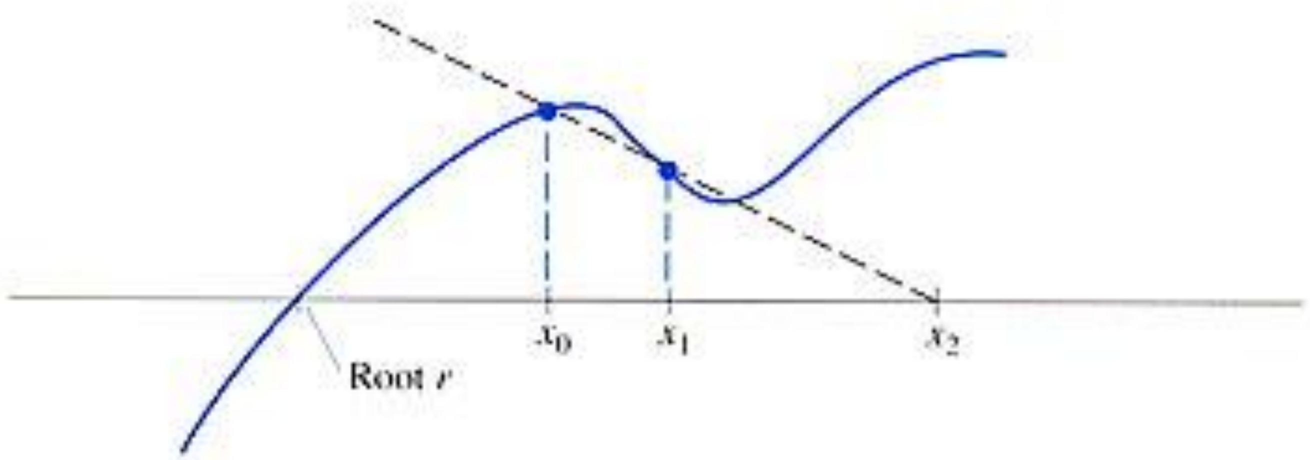


Figure 1.2
A pathological case for the secant method

False Position Method -1

- Avoid problems of secant method
  - Ensure that the root is bracketed between two starting values and remain between the successive pairs.
  - Similar to bisection method
    - x0 and x1 bracket a root

  Differences:

    - Next iterate is taken at the intersection of a line between the pair of x-values and the x-axis rather than the midpoint
    - Gives faster convergence than does bisection, but at expense of a more complicated algorithm

False Position Method -2

x_0 and x_1 bracket a root

Repeat

$$x_2 = x_1 - f(x_1)\frac{(x_0 - x_1)}{f(x_0) - f(x_1)}$$

if $f(x_2)$ opposite sign to $f(x_0)$

$x_1 = x_2$

else $x_0 = x_2$

Until $|f(x_2)| <$ tolerance value

Note:

if f(x) is not continuous, the method may fail.

A Comparison

- **Speed of convergence**
  - Secant (best), false position, then bisection

Table 1.3 Comparison of methods. $f(x) = 3x + \sin(x) - e^x = 0$, $x_0 = 0$, $x_1 = 1$

	Interval halving		False position		Secant method	
Iteration	x	$f(x)$	x	$f(x)$	x	$f(x)$
1	0.5	0.330704	0.470990	0.265160	0.470990	0.265160
2	0.25	−0.286621	0.372277	0.029533	0.372277	0.029533
3	0.375	0.036281	0.361598	$2.94 * 10^{-3}$	0.359904	$-1.29 * 10^{-3}$
4	0.3125	−0.121899	0.360538	$2.90 * 10^{-4}$	0.360424	$5.55 * 10^{-6}$
5	0.34375	−0.041956	0.360433	$2.93 * 10^{-5}$	0.360422	$3.55 * 10^{-7}$
Error after 5 iterations	0.01667		$-1.17 * 10^{-5}$		$< -1 * 10^{-7}$	

(Exact value of root is 0.360421703.)

Newton's Method -1

- Takes a single initial x_0 (not too far from a root), and the intersection of the tangent line and x-axis as the next
- Is the most widely used method
  - More rapidly convergent than bisection, secant and false position.

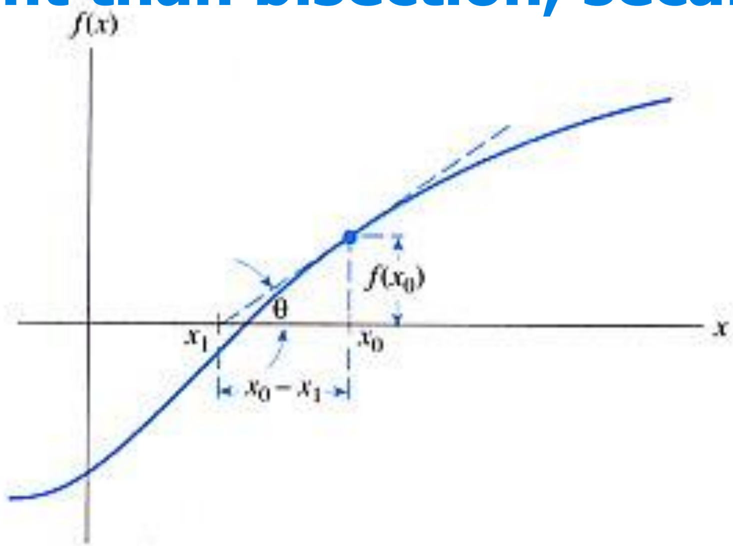


Figure 1.3

Newton's Method -2

- **Iteration**

$$\tan\theta = f'(x_0) = \frac{f(x_0)}{x_0 - x_1}$$

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$$

$$\vdots$$

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

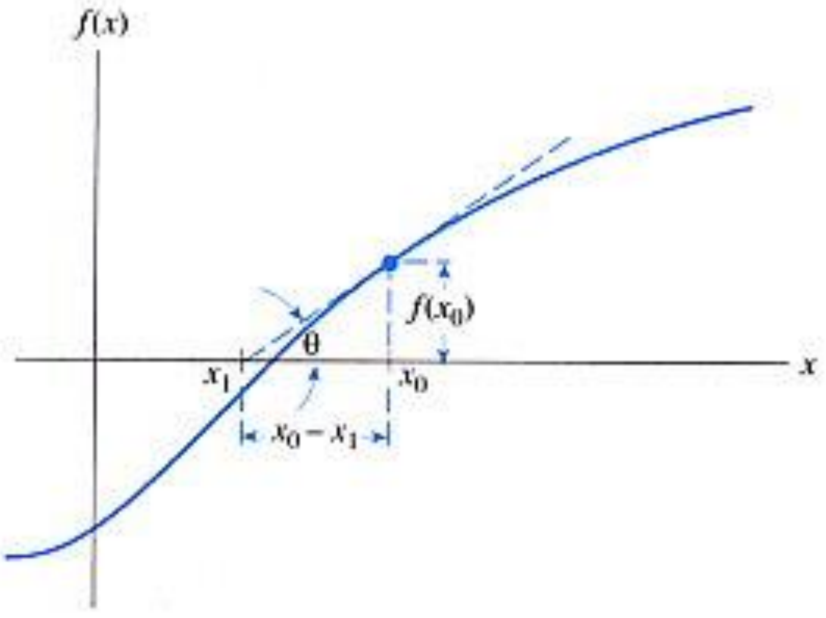


Figure 1.3

Newton's Method -3

Given a x_0 reasonably close to the root.

Compute $f(x_0)$ and $f'(x_0)$

if $(f(x_0) \neq 0)$ and $(f'(x_0) \neq 0)$

Repeat

$$x_1 = x_0$$

$$x_0 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

Until $(|x_0 - x_1| < \text{tolerance1})$ or

$(|f(x_0)| < \text{tolerance2})$

Note:

The method may converge to a root different from the expected one or diverge if the starting value is not close enough to the root.

Newton's Method -4

- Rate of convergence
  - Quadratically convergent
    - Error of each step approaches a constant K times the square of the error of the previous step
    - The net result of this is that the number of decimal places of accuracy nearly doubles at each iteration
    - Fewer steps than previous methods
      - But, at the cost of two function evaluations at each step
        - » Previous methods need only one at each step (after the first step)
    - Faster than any of the methods discussed so far

Newton's Method -5 - Example

$$f(x) = 3x + \sin x - e^x = 0$$

Starting with $x_0 = 0.0$

$x_1 = 0.33333$

$x_2 = 0.36017$

$x_3 = 0.3604217$

True $x = 0.360421703$

Note:

After 3 iterations, the solution is correct to 7 digits.

The error after an iteration is about 1/3 of the square of the previous error.

Newton's Method -6

- In some cases
  - May converge to a different root, diverge, or oscillating
    - Converge
    - Wandering: jump around, and then jump to a point near to the root, and then converge rapidly
    - In endless loop, i.e., cycling
      - Starting point near to an inflection point or a turning point (local minimum/maximum)
    - Overshooting
      - Fly off to infinity when ever reach the minimum or maximum of the curve
      - X-intercept x1 is far from both x0 and the desired root, may converge to different root

Newton's Method -7

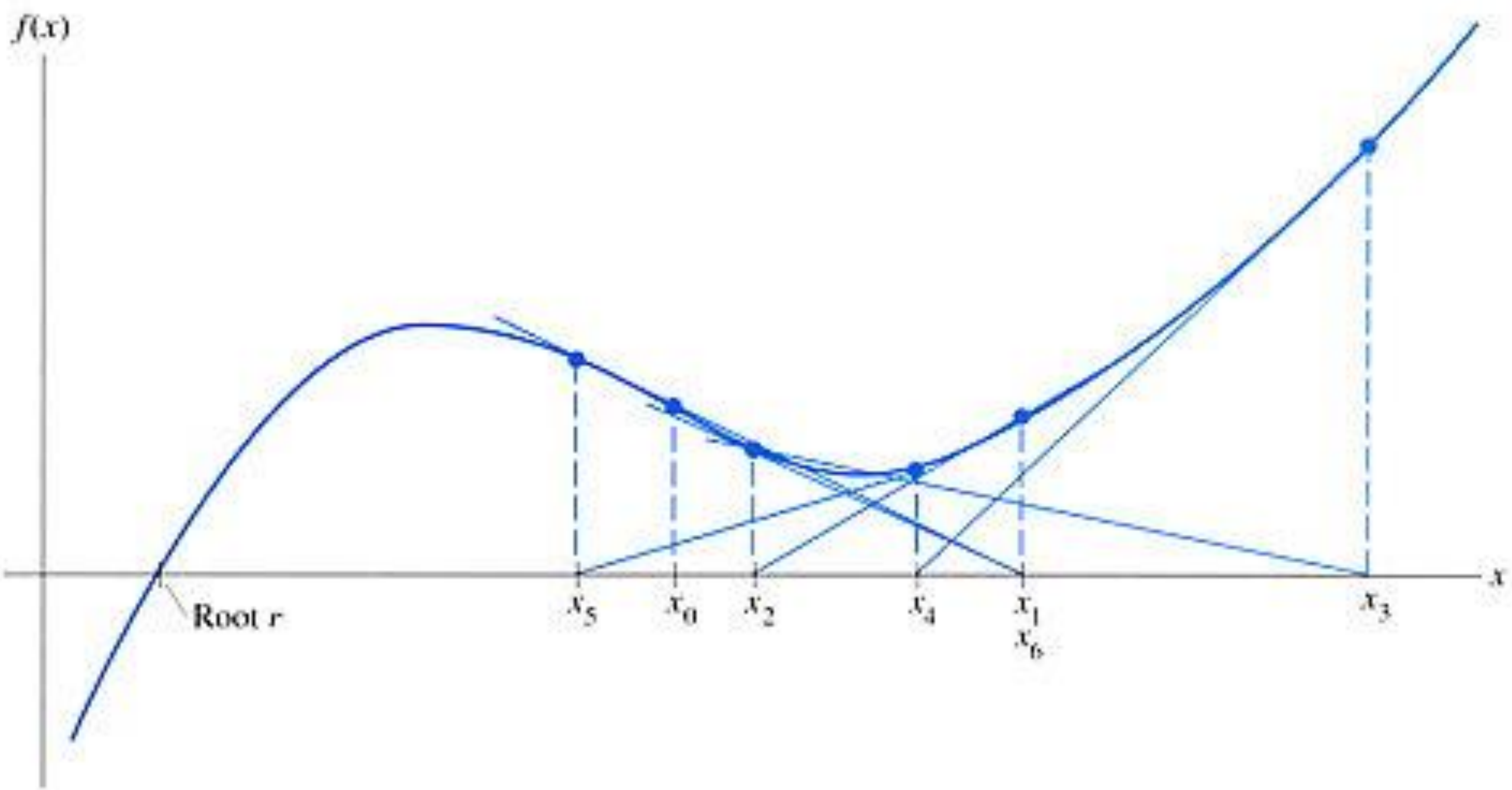


Figure 1.4

Starting point near to a turning point

Newton's Method -8 vs. interpolated methods

Interpolated methods :

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

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

Difference quotient approximates the derivative !! So closely resemble to Newton method!!

Newton's Method -9 Complex roots

- **Newton's method works with complex roots if a complex starting value is given.**

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

$f(x) = 0$ has a real root at $x = -3$

It has two complex roots because x-axis is not crossed again.

Start with $x_0 = 1 + i$, we have

$x_1 = 0.486238 + 1.04587i, x_2 = 0.448139 + 1.23665i$

$x_3 = 0.462720 + 1.22242i, x_4 = 0.462925 + 1.22253i$

$x_5 = 0.462925 + 1.22253i$

Since agree to 6 significan t digits, we have an estimate good to at least 6 significan t digits.

Start with $x_0 = 1 - i$, we have the conjugate $0.462925 - 1.22253i$

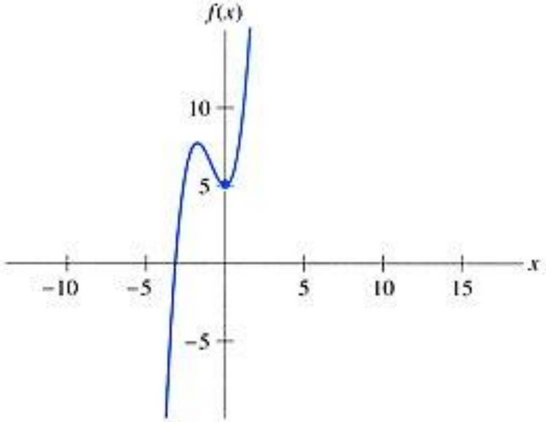


Figure 1.5
Plot of $f(x) = x^3 + 2x^2 - x + 5$

Newton's Method -10 for polynomials

- **Polynomials have nice behavior:**
  - They are everywhere continuous
  - They are smooth
  - Their derivatives are also continuous and smooth.
  - They are readily evaluated.
  - Number of roots can be predicted
  - Evaluation requires only +, -, *.

Newton's Method -11 for polynomials

- For previous methods, expect Newton method, there is nothing new (gain from the properties of polynomials)
- Polynomial evaluation of f(x) and f'(x) can be done by the use of **synthetic division**, which is based on the well known **remainder theorem**

Newton's Method -12 for polynomials

- **Evaluating a polynomial by nested form**
  - can be done by (or equivalent to) synthetic division
  - Evaluate f(x) at x=2

$$f(x) = 2x^3 + x^2 - 3x - 3$$
$$= ((2x+1)x-3)x-3$$
$$\Rightarrow \text{Process of synthetic division}$$

Synthetic division for $x = 2$:

$$\begin{array}{c|cccc} x=2 & 2 & 1 & -3 & -3 \\ & & 4 & 10 & 14 \\ \hline & 2 & 5 & 7 & 11 \end{array} \leftarrow \text{Remainder} = f(2)$$

Note: Nested form evaluation:

$$((2x+1)x-3)x-3$$

with x - 2: $((2\times 2+1)\times 2-3)\times 2-3 \rightarrow 11$

Remainder Theorem:

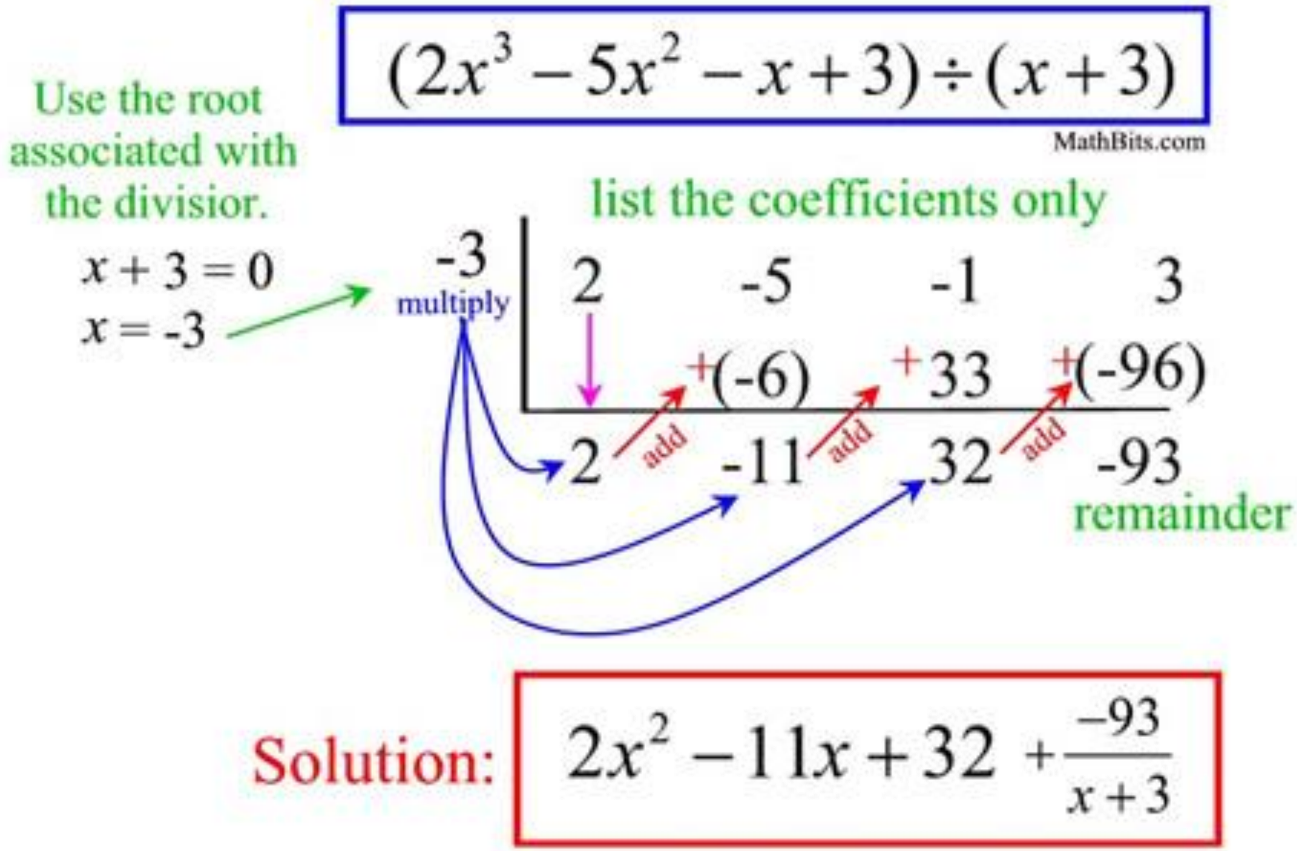
$$\frac{2x^3+x^2-3x-3}{x-2} = 2x^2+5x+7+\frac{11}{x-2}$$

That is,

$$2x^3+x^2-3x-3 = (x-2)(2x^2+5x+7)+11$$

Newton's Method -13 for polynomials

- **Example on synthetic division**



Newton's Method -14 for polynomials

- **If the reduced (quotient) polynomial is divided by x-2 again, the remainder is the value of the derivative at x=2**

$$f(x) = (x-2)(2x^2+5x+7)+11$$

$$f'(x) = (2x^2+5x+7)+(x-2)(4x+5)$$

$$\begin{array}{rrrr} x=2 & 2 & 5 & 7 \\ & & 4 & 18 \\ \hline & 2 & 9 & 25 \end{array} \leftarrow f'(2)$$

$f'(2)$ is the value of $2x^2+5x+7$ at $x=2$

$$f'(2) = 25$$

$$x_1 = 2 - \frac{11}{25} = 1.56$$

Newton's Method -15 for polynomials

Synthetic division algorithm :

A way of obtaining $Q_{n-1}(x)$ and R.

$$P_n(x) = a_n x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0$$

Reminder Theorem :

$$\begin{aligned} &P_n(x) \\ &= (x-a)Q_{n-1}(x) + R \\ &= (x-a)(b_{n-1}x^{n-1} + \cdots + b_1 x + b_0) + R \end{aligned}$$

Multiplying out and equating codfficients of like terms in x, we have

$$\left.\begin{aligned} a_n &= b_{n-1} \\ a_{n-1} &= b_{n-2} - ab_{n-1} \\ a_{n-2} &= b_{n-3} - ab_{n-2} \\ &\vdots \\ a_1 &= b_0 - ab_1 \\ a_0 &= R - ab_0 \end{aligned}\right\} \Rightarrow \left\{\begin{aligned} b_{n-1} &= a_n \\ b_{n-2} &= a_{n-1} + ab_{n-1} \\ b_{n-3} &= a_{n-2} + ab_{n-2} \\ &\vdots \\ b_0 &= a_1 + ab_1 \\ R &= a_0 + ab_0 \end{aligned}\right.$$

b_i and R are is the form of systhetic division

Newton's Method -16 for polynomials

- **If the quotient polynomial is divided by x-a again, the remainder is the value of the derivative at x=a. WHY?**

$$P_n(x) = a_n x^n + a_{n-1}x^{n-1} + \dots + a_1 x + a_0$$

Dividing $P_n(x)$ by x-a, we have

$$\frac{P_n(x)}{x-a} = Q_{n-1}(x) + \frac{R}{x-a}$$

That is,

$$P_n(x) = (x-a)Q_{n-1}(x) + R$$

So $P_n(a) = R$

Differentiate $P_n(x)$, we get

$$P_n'(x) = (x-a)Q_{n-1}'(x) + (1)Q_{n-1}(x)$$

Letting $x = a$, we have

$$P_n'(a) = Q_{n-1}(a) = \text{remainder on dividing } Q_{n-1}(x) \text{ by } (x-a).$$

Comparisons
Newton vs. secant

For simple root (i.e., f'(r)\=0)

- **Rate of convergence**
  - **Newton method: quadratically, order: 2**
  - **Secant method: order: 1.62**
    - **Faster than linear convergence**
  - **Both converge linearly to multiple roots**
- **Robustness**
  - **Newton method: converge, wandering, overshooting, and cycling**
  - **Secant method: converge, wandering, overshooting. But more robust than Newton**

Muller's method -1

- **A quadratic polynomial approximation is made to fit 3 points near a root.**

A quadratic polynomial $p_2(v) = av^2 + bv + c$

to fit $[x_1, f(x_1)],[x_0, f(x_0)],[x_2, f(x_2)]$

- **Using the quadratic rule to obtain the proper zero**

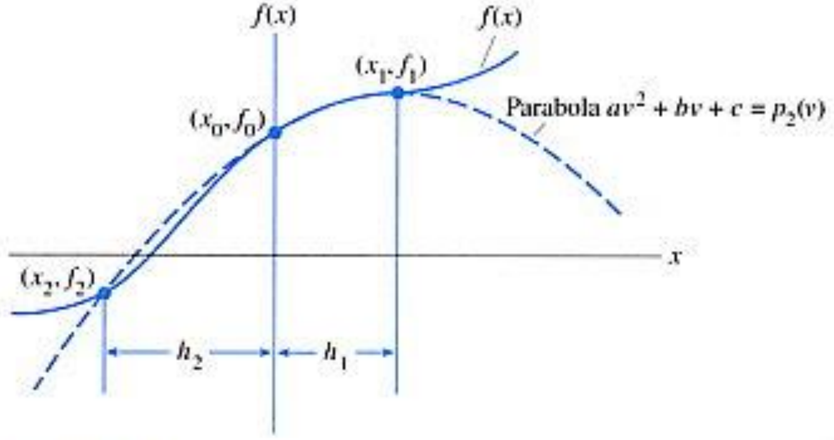


Figure 1.7

Muller's method -2

Simplify the development by transforming axes such that axes pass through the middle point.

So let $v = x - x_0$, and we try to fit the 3 points with $y = p_2(v) = av^2 + bv + c.$

Let $h_1 = x_1 - x_0, h_2 = x_0 - x_2,$

Evaluate the coefficients by evaluating $p(v)$ at the three points :

$v = 0: \quad a(0)^2 + b(0) + c = f_0 \Rightarrow c = f_0$

$v = h_1: \quad a(h_1)^2 + b(h_1) + c = f_1$

$v = -h_2: \quad a(h_2)^2 + b(-h_2) + c = f_2$

Let $\gamma = h_2/h_1$, solving two linear equations for a and b :

$$a = \frac{\gamma f_1 - f_0(1+\gamma) + f_2}{\gamma h_1^2 (1+\gamma)}$$

$$b = \frac{f_1 - f_0 - a h_1^2}{h_1}$$

Muller's method -3

- Solve for the root of $p_2(v) = av^2 + bv + c = 0$ by the quadratic formula, **choosing the root nearest to the middle point x_0 by making the absolute value of denominate as large as possible** in the following form:

$$\text{root} = x_0 - v = x_0 - \frac{2c}{b \pm \sqrt{b^2 - 4ac}} \left(= x_0 + \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \right)$$

  - WHY? See next slide
    - More stable compared to standard one
    - Choose the sign to give the largest absolute value of denominator: b>0: +, b<0: --, b=0: either

Muller's method -4

$$p_2(v) = av^2 + bv + c$$
$$= a(x - x_0)^2 + b(x - x_0) + c = 0$$
$$v = x - x_0 = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$\boxed{\begin{array}{l} x = x_0 + \dfrac{-b \pm \sqrt{b^2 - 4ac}}{2a} \\ \text{with } \pm \text{ chosen to minimize the modulus} \\ \text{of the numerator (} x \text{ is closest to } x_0\text{):} \\ \text{b} > 0 \text{ --> take } +, \text{ b} < 0 \text{ --> take } -. \end{array}}$$

But minimizing the numerator may cancel significan t digits when b^2 is much larger than $4ac$ (since $\sqrt{b^2 - 4ac} \sim b$).

Example:

$p(v) = v^2 + 62.10v + 1 = 0$

Using 4-digit rounding arithmetic

$b > 0$, so take $+$,

$\sqrt{b^2 - 4ac} = 62.06 \approx b = 62.10$

and $x_1 = -0.01610723$,

with relative error: 2.4×10^{-1}

cancellation error → Large error!

Other root:

$x_2 = -62.08390$,

with relative error: 3.2×10^{-4}

Muller's method -5

Equivalent form:

$$\left(\frac{-b+\sqrt{b^2-4ac}}{2a}\right)\left(\frac{-b-\sqrt{b^2-4ac}}{-b-\sqrt{b^2-4ac}}\right)$$

$$=\frac{b^2-(b^2-4ac)}{2a(-b-\sqrt{b^2-4ac})}=\frac{-2c}{b+\sqrt{b^2-4ac}}$$

$$\left(\frac{-b-\sqrt{b^2-4ac}}{2a}\right)\left(\frac{-b+\sqrt{b^2-4ac}}{-b+\sqrt{b^2-4ac}}\right)$$

$$=\frac{-2c}{b-\sqrt{b^2-4ac}}$$

To guard against this, root is calculated in the equivalent form:

$$x = x_0 - \frac{2c}{b \pm \sqrt{b^2-4ac}}$$

with $\pm$ chosen to maximize the modulus of the denominator:

$b > 0$ --> take $+$

$b < 0$ --> take $-$

There will be no case of substracting two nearly equal numbers.

Muller's method -6

Using the equivalent form:

$$x = x_0 - \frac{2c}{b \pm \sqrt{b^2 - 4ac}}$$

$b > 0$, take $+$

$x_1 = -0.01610,$

relative error: 6.2×10^{-4}

No cancellation error → Smaller error!

Other root:

$x_2 = -50.00,$

relative error: 1.9×10^{-1}

Muller's method -7

- Start from three initial point x1, x0, x2
- Find a quadratic form passing through three point and find the roots
- Choose next 3 points that are **most closely spaced**
  - The root is to the right of x_0: x_0, x_1, root
  - The root is to the left of x_0 : x_0, x_2, root

Muller's method -8

Procedure:

Given points $x_2 < x_0 < x_1$,

- Evaluate the functions f_2, f_0, f_1.
- Find the coefficients of $p_2(v)$.
- Compute the roots:

$$x_r = x_0 - \frac{2c}{b \pm \sqrt{b^2 - 4ac}}$$

Choose the root closest to x_0

by making the denominator as largeas possible, and label it x_r

If $x_r > x_0$

then rearrange to x_0, x_1, x_r

else rearrange to x_0, x_2, x_r

Until $\left| f(x_r) \right| < \text{Ftol}$

Muller's method -9

- Converge rate: similar to that for Newton method (actually order 1.85)
- No derivative evaluation and only one function evaluation per iteration (after we have obtained the next point)
- Will find a complex root if complex starting value is given
- May fail under some conditions
  - What will make the denominator of root's expression zero or nearly zero

Muller's method -10

EXAMPLE 1.2 Find a root between 0 and 1 of the same transcendental function as before: $f(x) = 3x + \sin(x) - e^x$. Let

$$
\begin{aligned}
x_0 &= 0.5, & f(x_0) &= 0.330704 & h_1 &= 0.5,\\
x_1 &= 1.0, & f(x_1) &= 1.123189 & h_2 &= 0.5,\\
x_2 &= 0.0, & f(x_2) &= -1 & \gamma &= 1.0.
\end{aligned}
$$

Then

$$a = \frac{(1.0)(1.123189) - 0.330704(2.0) + (-1)}{1.0(0.5)^2(2.0)} = -1.07644,$$

$$b = \frac{1.123189 - 0.330704 - (-1.07644)(0.5)^2}{0.5} = 2.12319,$$

$$c = 0.330704,$$

and

$$\text{root} = 0.5 - \frac{2(0.330704)}{2.12319 + \sqrt{(2.12319)^2 - 4(-1.07644)(0.330704)}}$$

$$= 0.354914.$$

Muller's method -10

For the next iteration, we have

$$
\begin{aligned}
x_0 &= 0.354914, & f(x_0) &= -0.0138066 & h_1 &= 0.145086,\\
x_1 &= 0.5, & f(x_1) &= 0.330704 & h_2 &= 0.354914,\\
x_2 &= 0, & f(x_2) &= -1 & \gamma &= 2.44623.
\end{aligned}
$$

Then

$$a = \frac{(2.44623)(0.330704) - (-0.0138066)(3.44623) + (-1)}{2.44623(0.145086)^2(3.44623)} = -0.808314,$$

$$b = \frac{0.330704 - (-0.0138066) - (-0.808314)(0.145086)^2}{0.145086} = 2.49180,$$

$$c = -0.0138066,$$

$$\text{root} = 0.354914 - \frac{2(-0.0138066)}{2.49180 + \sqrt{(2.49180)^2 - 4(-0.808314)(-0.0138066)}}$$

$$= 0.360465.$$

After a third iteration, we get 0.3604217 as the value for the root, which is identical to that from Newton's method after three iterations. ▲

Fixed-Point Iteration -1

- **A useful way for root finding**
- **Basis for some important theory**
- **Fixed point** $f(x)=0 \Rightarrow x=g(x)$ (in several forms)

  r : a fixed point of g if $r=g(r)$
- **Fixed-point iteration** $x_{n+1}=g(x_n), \quad n=0,1,2,3,\ldots$
- **Under *suitable conditions*, the fixed-point iteration converges to the fixed point r, a root of f(x)=0**
- **Different rearranges will converge at different rate, or converge to different root, or diverge**

Fixed-Point Iteration -2

$f(x) = x^2 - 2x - 3 = 0 \quad \text{roots}: -1, 3$

1. $x = g_1(x) = \sqrt{2x+3}$

   Start with $x_0 = 4$:

   $x_1 = 3.31662, \ x_2 = 3.10375$

   $x_3 = 3.03439, \ x_4 = 3.01144$

   $x_5 = 3.00381 \Rightarrow$ converges to $x = 3$

2. $x = g_2(x) = \dfrac{3}{x-2}$

   $x_1 = 1.5, \ x_2 = -6, x_3 = -0.375,$

   $x_4 = -1.263158, \ x_5 = -0.919355$

   $x_6 = -1.02762, \ x_7 = -0.990876$

   $x_8 = -1.00305 \ \Rightarrow$ converges to $x = -1$

3. $x = g_3(x) = \dfrac{x^2-3}{2}$

   $x_0 = 4,$

   $x_1 = 6.5$

   $x_2 = 19.625,$

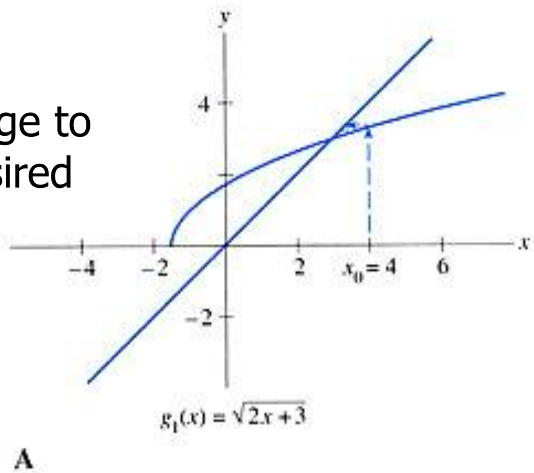
   $x_3 = 191.070 \Rightarrow$ diverges

Different arrangements have different convergence behavior. Why?

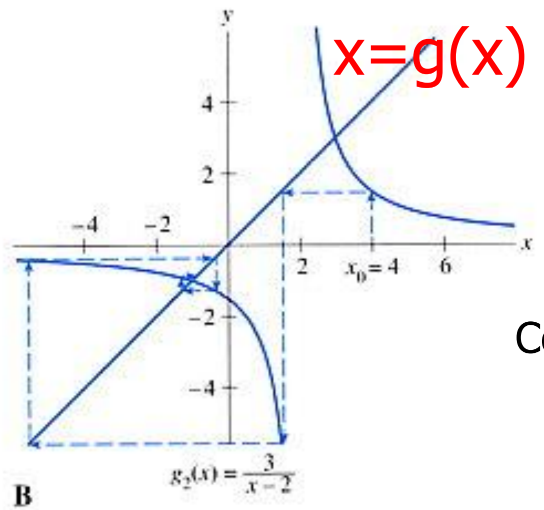
Look into this problem by using the graph of two intersecting plots of $y = x$ and $y = g(x)$.

Fixed-Point Iteration -3

Converge to the desired root



$x=g(x) \Leftrightarrow y=x$ and $y=g(x)$



Converge to another root

Diverge!

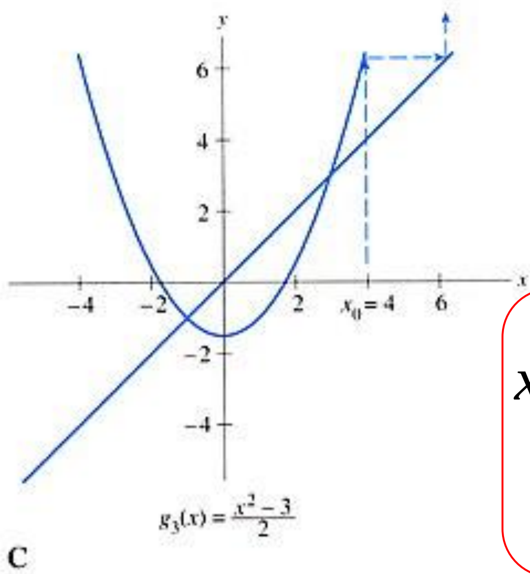


Figure 1.8

$$x_k \xrightarrow{g(x_k)} x_{k+1}$$

$$x_k \xrightarrow[\text{to the graph of } g]{\text{move up or down}} P_k \xrightarrow[\text{to the graph of } y=x]{\text{move right or left}} Q_{k+1} \xrightarrow[\text{to the } x\text{-axis}]{\text{move up or downt}} x_{k+1}$$

$$g(x_k) \qquad y = g(x_k) \qquad x_{k+1} = y = g(x_k)$$

Fixed-Point Iteration -4
Rate of Convergence

Assume $\{x_n\}_{n=0}^{\infty}$ converges to r.

Let $e_n = x_n - r$.

If $|e_n|$ approaches to $c|e_{n-1}|^k$ as n becames infinite, we say that the sequence converges to r with order of convergence k, or formally :

The sequence $\{x_n\}_{n=0}^{\infty}$ is called linearly converge to r if $e_n \to 0$ in such a way that

$$\lim_{n\to\infty} \frac{e_n}{e_{n-1}} = C_L, \text{ where } 0 < |C_L| < 1$$

The sequence $\{x_n\}_{n=0}^{\infty}$ is called superlinearly converge to r if $e_n \to 0$ in such a way that

$$\lim_{n\to\infty} \frac{e_n}{e_{n-1}} = 0$$

The sequence $\{x_n\}_{n=0}^{\infty}$ is called quadratically convergeto r if $e_n \to 0$ in such a way that

$$\lim_{n\to\infty} \frac{e_n}{e_{n-1}{}^2} = C_Q, \text{ where } C_Q \neq 0$$

Fixed-Point Iteration -5

$x_{n+1} = g(x_n)$ and r is the root (fixed point)

- **Error**

  e_{n+1} and e_n

$$x_{n+1} - r = g(x_n) - r = \frac{g(x_n) - g(r)}{x_n - r}(x_n - r)$$

If $g(x)$ and $g'(x)$ are continuous on the interval from r to x_n, the mean value theorem implies that

$$x_{n+1} - r = g'(\tau_n)(x_n - r),$$

where τ_n lies between x_n and r, and hence

$$|\mathrm{e}_{\mathrm{n+1}}| = |g'(\tau_n)||e_n|$$

- **Condition for convergence**

Suppose $|g'(x)| < K < 1$ for all x in the interval of size h around the root.

If x_0 is chosen in this interval, fixed point iteration will converge because

$$|e_{n+1}| < K|e_n| < K^2|e_{n-1}| < \cdots < K^{n+1}|e_0|.$$

Note that all succeeding iterates will lie in this interval and will converge to r.

Fixed-Point Iteration -6 Convergence Rate

- **Order of convergence: linear**

$$\begin{aligned}|e_{n+1}| &= |x_{n+1} - r| \\ &= |g'(\tau_n)(x_n - r)| \\ &= |g'(\tau_n)||e_n|,\end{aligned}$$

where τ_n lies between x_n and r.

So if $|g'(x)| < K < 1$ for all x in the interval,

$$\lim_{n\to\infty}\frac{|e_{n+1}|}{|e_n|} = \lim_{n\to\infty}|g'(\tau_n)|, \text{where } \tau_n \text{ lies between } x_n \text{ and } r.$$

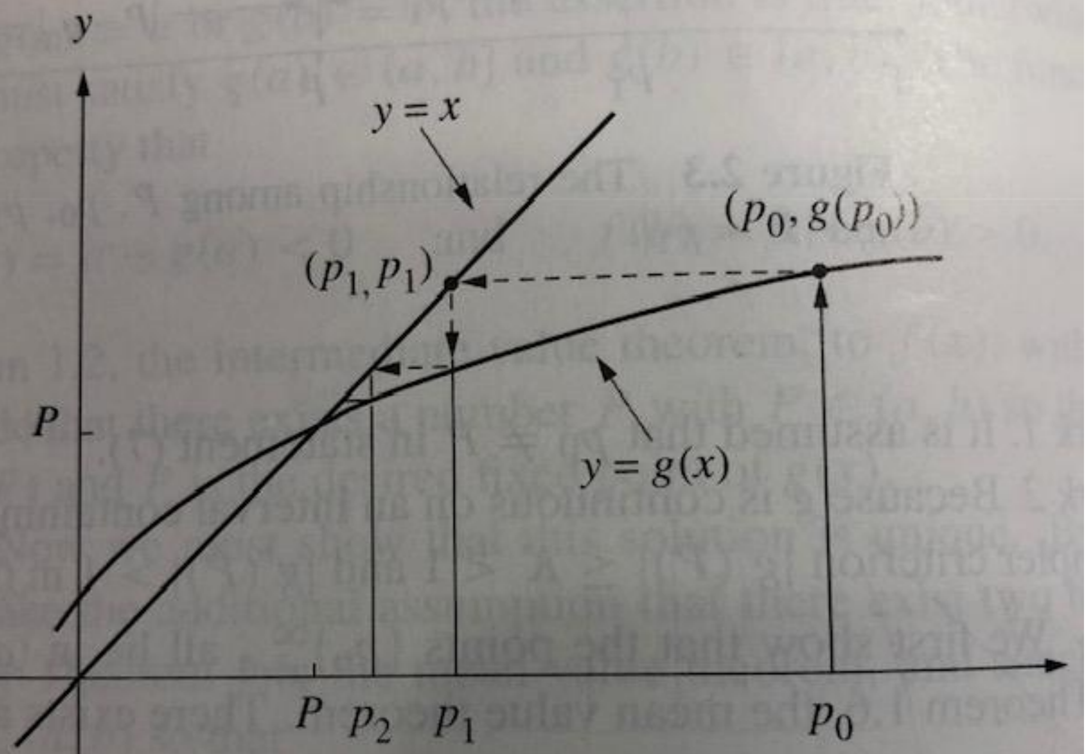
$$= |g'(r)| < 1 \text{ (since } x_n \text{ converges to } r, \tau_n \text{ converges to } r\text{)}$$

Converge linearly!

Fixed-Point Iteration -7

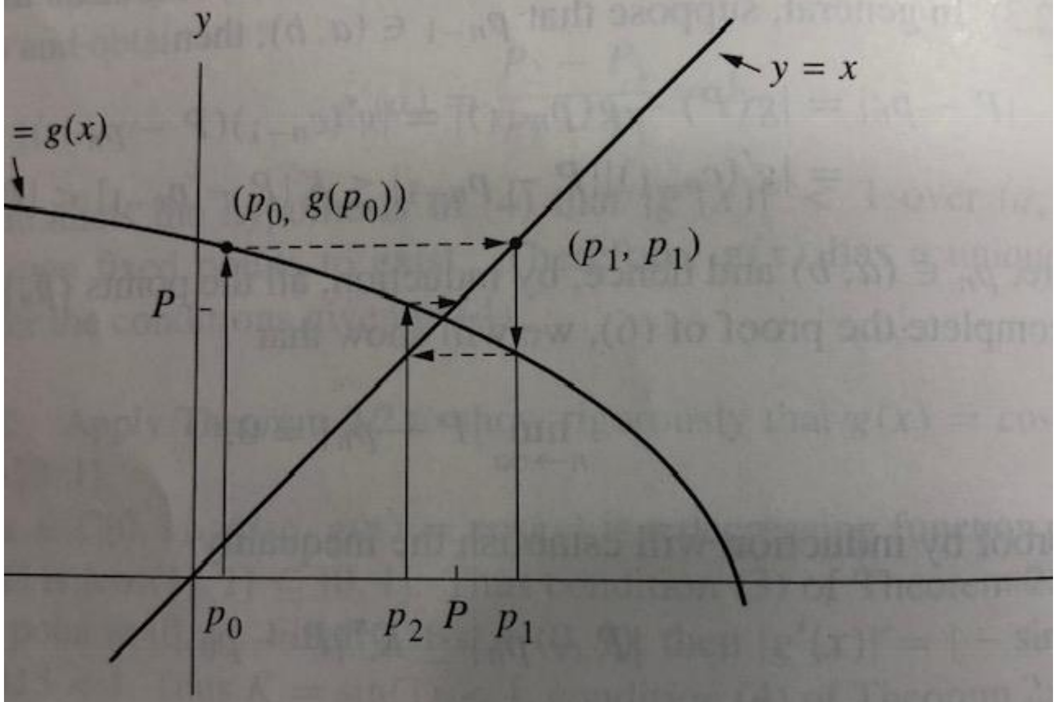
- Converge $|g'(p)| < 1$
  - Monotone converging
    - $0 < g'(p) < 1$
  - Oscillating converging
    - $-1 < g'(p) < 0$
- Diverge $|g'(p)| > 1$
  - Monotone diverging
    - $1 < g'(p)$
  - Oscillating diverging
    - $g'(p) < -1$

Fixed-Point Iteration -9



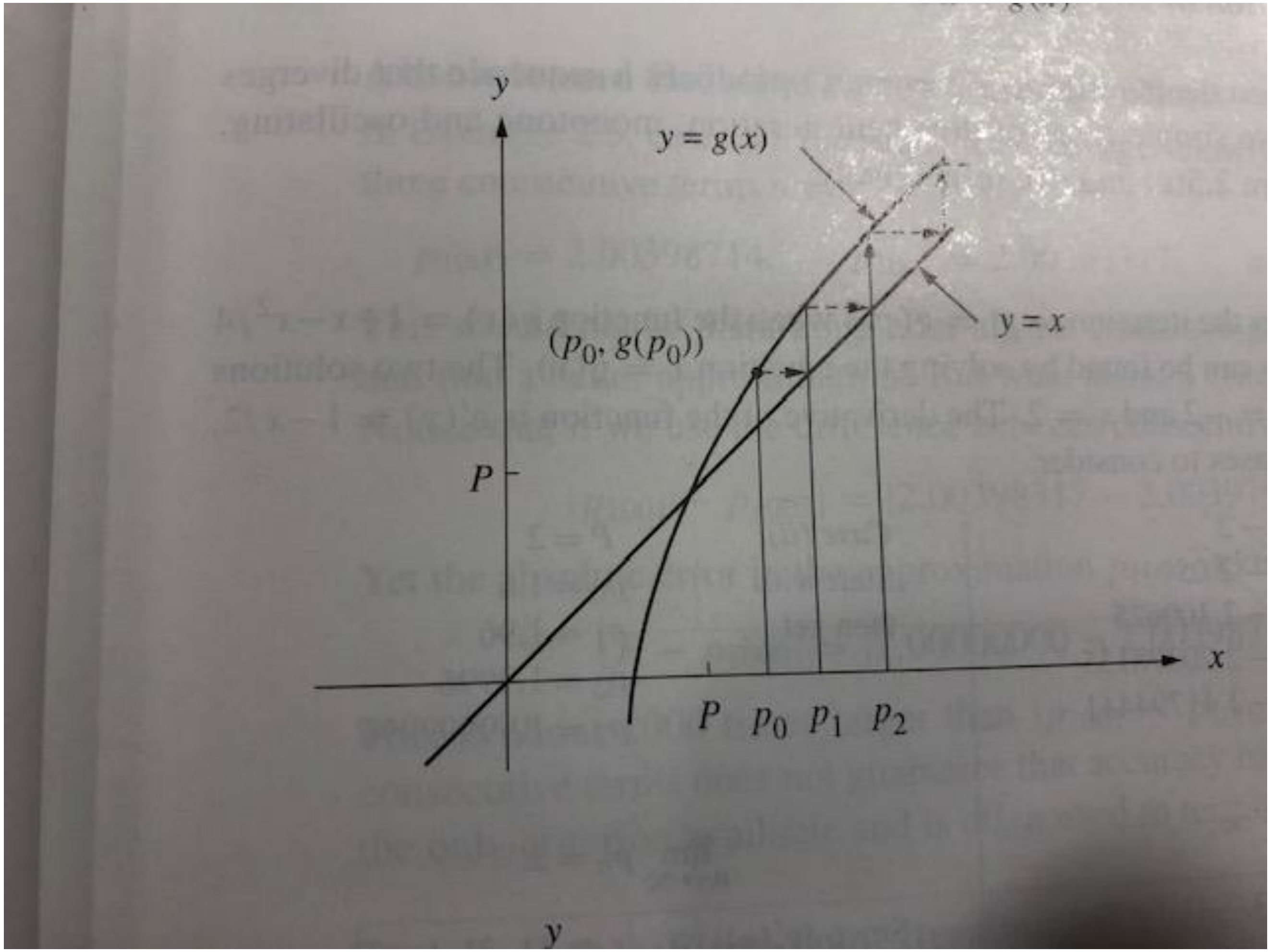
igure 2.4 (a) Monotone convergence when $0 < g'(P) < 1$.

Fixed-Point Iteration -8



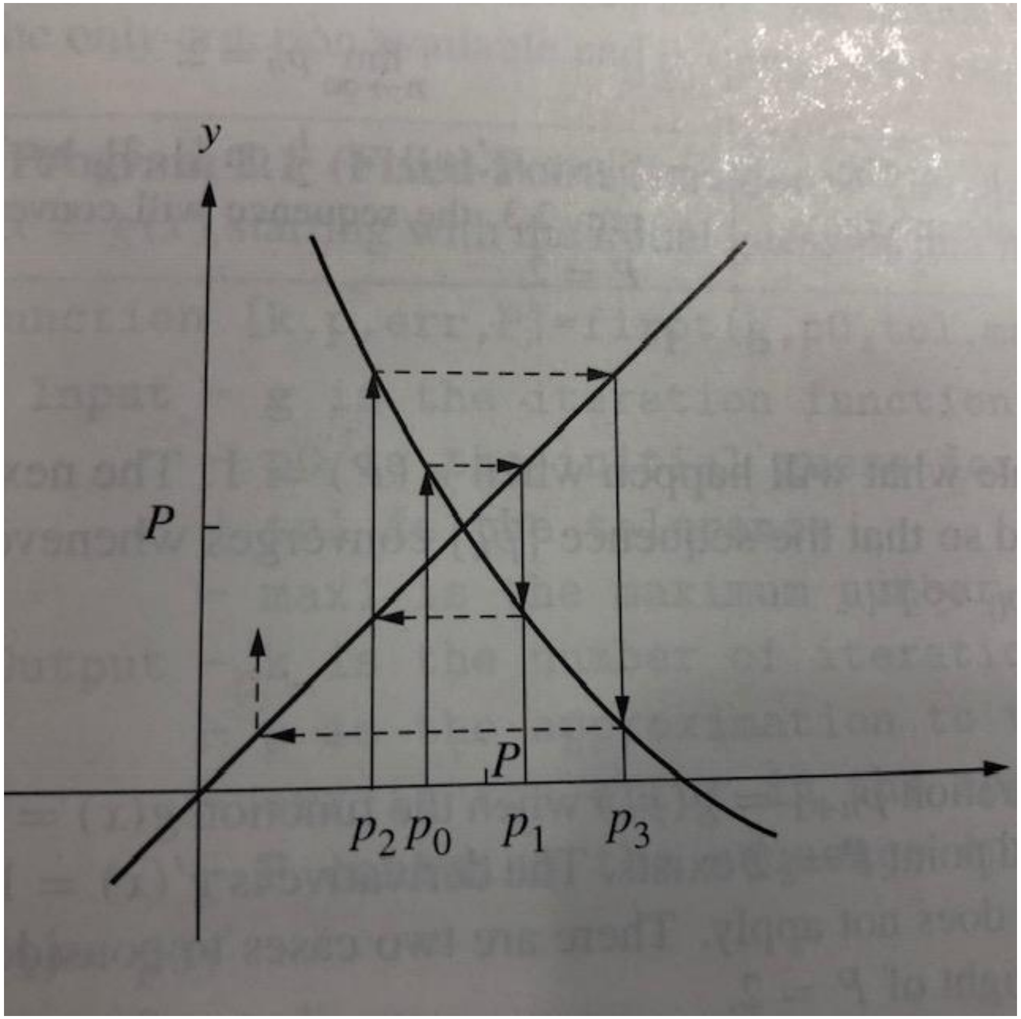
gure 2.4 (b) Oscillating convergence when $-1 < g'(P) < 0$.

Fixed-Point Iteration -10



1<g′(x) : Monotone divergent

Fixed-Point Iteration -11



g′(x) < -1: Oscillating divergent

Convergence Condition for Newton Method

Rewrite the Newton method as a fixed-point iteration :

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = g(x_n)$$

$$g'(x) = \frac{f(x) f''(x)}{\left[f'(x)\right]^2}$$

Based on the condition for convergence of fixed-point iteration :

Newton method converges if, on an interval about the root r,

$$\left|g'(x)\right| = \left|\frac{f(x) f''(x)}{\left[f'(x)\right]^2}\right| < 1$$

provided that x_0 is in the interval.

Convergence Order for Newton Method (for simple root)

By Taylor expansion of $g(x)$ at r:

$$g(x) = g(r) + g'(r)(x-r) + \frac{g''(\xi)}{2}(x-r)^2$$

where ξ lies in the interval from x_n to r.

Since $f(r)=0$, $g'(r) = \dfrac{f(r)f''(r)}{[f'(r)]^2} = 0$,

we have

$$g(x_n) = g(r) + \frac{g''(\xi_n)}{2}(x_n - r)^2$$

$$e_{n+1} = x_{n+1} - r = g(x_n) - g(r) = \frac{g''(\xi_n)}{2} e_n{}^2$$

As the iterates x_n approach to r when n approaches to infinity, so does ξ_n. That is,

$$\lim_{n\to\infty} \frac{|e_{n+1}|}{|e_n|^2} = \lim_{n\to\infty} \left| \frac{g''(\xi_n)}{2} \right| = \left| \frac{g''(r)}{2} \right| \neq 0$$

(for simple root)

So Newton method is quadratically convergent.

Convergence Condition of Bisection Method

- **[From Mathews and Fink, p 54]**

Theorem

Assume that $f \in C[a,b]$ and that there exists a number $r \in [a,b]$ such that $f(r)=0$. If $f(a)f(b)<0$, the sequence $\{x_n\}_{n=0}^{\infty}$ generated by the bisection process, then

$$|x_n - r| \le \frac{b-a}{2^{n+1}} \quad \text{for } n = 0,1,2,\ldots$$

Therefore

$$\lim_{n\to\infty} x_n = r.$$

Convergence Condition of Bisection Method

Pf : Since the root r and midpoint x_n lie in [a, b],

$$|x_n - r| \le \frac{b_n - a_n}{2}, \text{ for all } n.$$

Observe that $b_1 - a_1 = \dfrac{b_0 - a_0}{2}$ $\quad (a_0 = a, b_0 = b)$

$$b_2 - a_2 = \frac{b_1 - a_1}{2} = \frac{b_0 - a_0}{2^2}$$

By induction, we have

$$b_n - a_n = \frac{b_0 - a_0}{2^n}$$

So

$$|x_n - r| \le \frac{b_n - a_n}{2} \le \frac{b_0 - a_0}{2^{n+1}}$$

Convergence Condition of Bisection Method

Proof by induction:
Basic step: prove it is true for **n=1**
Induction step:
Assume it is true for **n=k**
Prove it is true for **n=k+1**

Pf : Since the root r and midpoint x_n lie in [a, b],

$$|x_n - r| \le \frac{b_n - a_n}{2}, \text{ for all } n.$$

Basic step : Observe that $b_1 - a_1 = \dfrac{b_0 - a_0}{2}$ $\quad (a_0 = a, b_0 = b)$

$$b_2 - a_2 = \frac{b_1 - a_1}{2} = \frac{b_0 - a_0}{2^2}$$

Induction step : Assuning it is true for n-1, we have

$$b_n - a_n = \frac{b_{n-1} - a_{n-1}}{2} = \frac{1}{2}\frac{b_0 - a_0}{2^{n-1}} = \frac{b_0 - a_0}{2^n}$$

So

$$|x_n - r| \le \frac{b_n - a_n}{2} \le \frac{b_0 - a_0}{2^{n+1}}$$

Convergence Order of Bisection Method

- **One-half of the current interval is an upper bound to the error, which can serve as the estimate of the error**
- **So $|e_{n+1}|=0.5\ |e_n|$ Linearly convergent!!**

Since

$$e_{n+1}=\left|x_{n+1}-r\right|\le\frac{b_{n+1}-a_{n+1}}{2},\quad e_{n+1}\approx\frac{b_{n+1}-a_{n+1}}{2}$$

$$e_n=\left|x_n-r\right|\le\frac{b_n-a_n}{2},\ e_n\approx\frac{b_n-a_n}{2}$$

$$\lim_{n\to\infty}\frac{e_{n+1}}{e_n}=\left(\frac{b_{n+1}-a_{n+1}}{2}\right)/\left(\frac{b_n-a_n}{2}\right)=\frac{1}{2}$$

$$(\text{since } b_{n+1}-a_{n+1}=\frac{b_n-a_n}{2})$$

Convergence Order of Secant Method

Consider $x_{n+1} = g(x_n, x_{n-1})$.

Apply Taylor series and derive

$$\lim_{n=0}^{\infty} \frac{|e_{n+1}|}{|e_n e_{n-1}|} = \frac{1}{2}\left|\frac{f''(r)}{f'(r)}\right|$$

Further error analysis leads to

$$\lim_{n\to\infty} \frac{|e_{n+1}|}{|e_n|^{\alpha}} = K,$$

where

$$\alpha = \frac{1+\sqrt{5}}{2} = 1.62,\ \ K = \frac{1}{2}\left|\frac{f''(r)}{f'(r)}\right|^{1/\alpha}$$

So convergence order is 1.618.

Convergence Order for All Methods: summary

- **Fixed-point iteration: Order: linear**
- **Bisection: Order: linear**
  - One-half of the current interval is an upper bound to the error, which can serve as the estimate of the error
  - So $|e_{n+1}|=0.5\ |e_n|$
- **False Position: Order: linear**
  - $X_{n+1}=g(x_n, x_{n-1})$
  - The root is always bracketed, so x_{n-1} can be thought as a constant
  - It is exactly as the fixed-point iteration, so it is linearly convergent

Convergence order for All Methods : summary

- **Secant method: order: 1.62**
  - $x_{n+1}=g(x_n, x_{n-1})$
  - Similar analysis as the Newton method results in

$$e_{n+1} = \frac{g''(\xi_1)g''(\xi_2)}{2} e_n e_{n-1}$$

  - Better than linear convergence but poorer than quadratic convergence. It has been shown the order is 1.62.
- **Muller method: order=1.85**
- **Newton method: order= 2 (quadratic)**

Starting Point Issues

- **Newton method requires the initial point to be close to a root. General cases:**
  - Converge, or scattering and then converge (wandering)
  - Oscillating
  - Diverge
- **Newton method for polynomials (all roots)**
  - Obtain an approximate for the first root
  - Proceed to obtain additional roots from the reduced polynomial, in which synthetic division can be employed to improve an initial estimate.
  - The process is repeated until the reduced polynomial is of degree 2

Multiple Roots -1

- **Multiple roots**
  - **Examples**
    - $f(x)=(x+1)^3$: triple root at $x=-1$
    - $f(x)=(x-2)^2$: double root at $x=2$

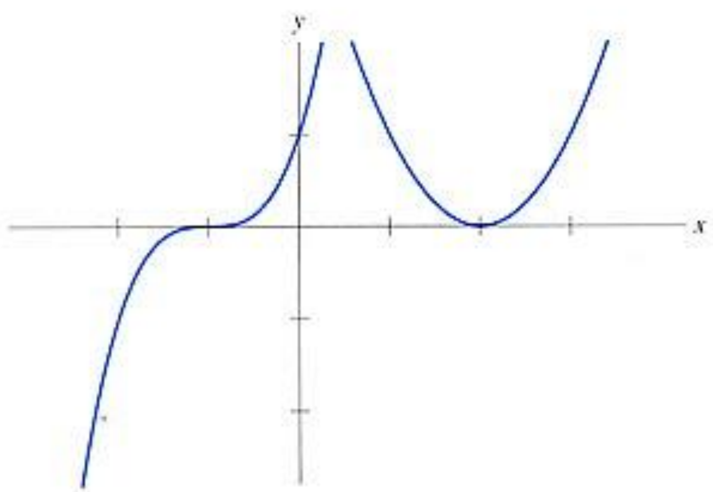


Figure 1.9

Multiple Roots -2

Previous methods do not work well

- **Newton/secant method converges only linearly to a double/triple root**
- **Bisection and false position methods fail to get a double root. (because no sign changes)**
- **Muller's method is fastest, then Newton method, and then Secant method**

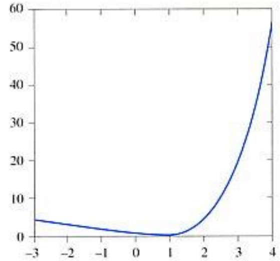


Figure 1.10
Plot of $(x-1)(e^{(x-1)}-1)$

Table 1.7 Getting a double root, for $f(x) = (x-1) * (e^{(x-1)} - 1)$

	Secant method	Newton's method	Muller's method
Estimate after 9 iterations	1.00331	1.00126	1.00058
Start value(s)	1.2, 1.5	2.0	0, 1.2, 1.5

Double root at 1

Multiple Roots -3

- **Problems for Newton method**
  - Slow convergence: Converge linearly at double/triple roots with ratio (k-1)/k
    - Ratio of errors=1/2 for double roots
    - Ratio of errors=2/3 for triple roots
  - Another disadvantage: Imprecision
    - Curve is flat near the root
      - f'(x) will always be 0 at a root
      - There is a "neighborhood of uncertainty" around the root, where f(x) are very small around the root
        - » Computers will find f(x) equal to 0 throughout the neighborhood of the root
        - » Program cannot distinguish which value is really the root
        - » Using double precision helps to decrease the neighborhood of uncertainty

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

Multiple Roots -4

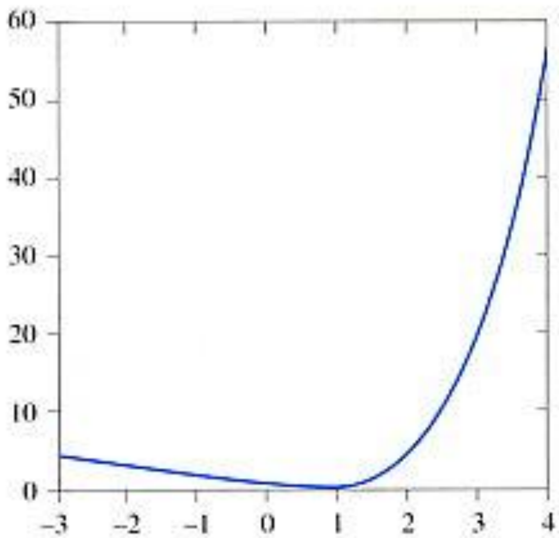


Figure 1.10
Plot of $(x-1)(e^{(x-1)}-1)$

Table 1.4 Errors when finding a double root

Iteration	Error	Ratio
1	0.3679	
2	0.1666	0.453
3	0.0798	0.479
4	0.0391	0.490
5	0.0193	0.494
6	0.0096	0.497
7	0.0048	0.500
8	0.0024	0.500

Converge linearly to a double root with ratio=1/2

Multiple Roots -5

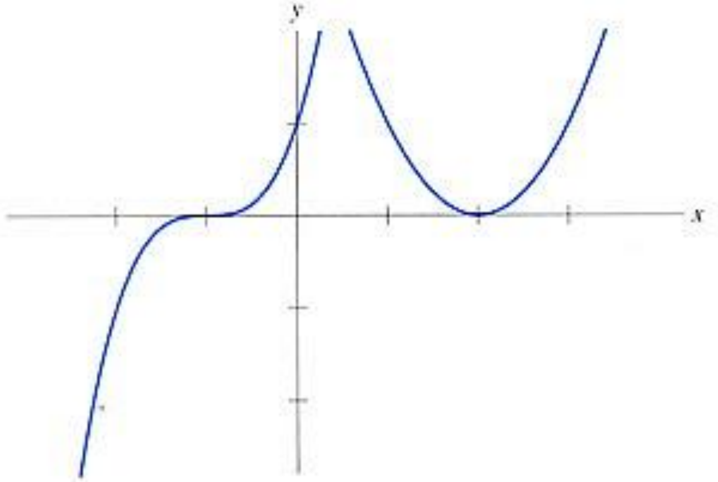


Figure 1.9

Table 1.10 Successive errors with Newton's method, for $f(x) = (x+1)^3 = 0$

Iteration	Error	Iteration	Error
0	0.5	6	0.0439
1	0.3333	7	0.0293
2	0.2222	8	0.0195
3	0.1482	9	0.0130
4	0.0988	10	0.00867
5	0.0658		

Converge linearly to a triple root with ratio=2/3

Multiple Roots -6

- Linear convergence of Newton method to a double root and triple root
- For double roots
  - Bisection/false position methods fail for double roots
- For triple roots
  - All methods work, but even slower

Multiple Roots -7

- **Why linearly converge with error ratio (k-1)/k?**

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = g(x_n)$$

Taylor series of $g(x)$ about r:

$$g(x) = g(r) + g'(r)(x-r) + (g''(\xi)/2)(x-r)^2$$

For simple roots, $g'(r) = 0$ leads to quadratic convergence.

For a root r of multiplicity k,

$$\boxed{\text{we cannot say } g'(r) = \frac{f(r)f''(r)}{\left(f'(r)\right)^2} = 0. \text{ Why? } \quad 0/0}$$

We can factor out $(x-r)^k$ from $f(x)$ to get

$$f(x) = (x-r)^k Q(x), \text{ where } Q(r) \neq 0,$$

even though $f'(r) = f''(r) = \ldots\ldots = f^{(k-1)}(r) = 0.$

Multiple Roots -8

Consider $g'(x) = \dfrac{f(x) f''(x)}{[f'(x)]^2}$ and let $h = x - r$

$g'(x)$

$$= \frac{h^k Q(x)\left[h^k Q''(x) + 2kh^{k-1}Q'(x) + k(k-1)h^{k-2}Q(x)\right]}{\left[h^k Q'(x) + kh^{k-1}Q(x)\right]^2}$$

$$= \frac{h^{2k-2} Q(x)\left[h^2 Q''(x) + 2khQ'(x) + k(k-1)Q(x)\right]}{h^{2k-2}\left[hQ'(x) + kQ(x)\right]^2}$$

When $x = r$, both denominator and numerator are 0, we cannot say $g'(r) = 0$.

Actually dividing denominator and numerator by h^{2k-2}, we have

$$\lim_{h\to 0} g'(x) = g'(r)$$

$$= \frac{Q(r)\left[0\cdot Q''(r) + 0\cdot Q'(r) + k(k-1)Q(r)\right]}{\left[0\cdot Q'(r) + kQ(r)\right]^2}$$

$$= \frac{k(k-1)Q(r)^2}{k^2 Q(r)^2} = \frac{k-1}{k} \neq 0$$

$$g(x_n) = g(r) + g'(\xi_n)(x_n - r)$$

$$e_{n+1} = x_{n+1} - r = g(x_n) - g(r) = g'(\xi_n)e_n$$

$$\lim_{n\to\infty} \frac{|e_{n+1}|}{|e_n|} = \lim_{n\to\infty} g'(\xi_n) = g'(r) = \frac{k-1}{k}.$$

So the convergence is linear with

$$\lim_{n\to\infty} \frac{|e_{n+1}|}{|e_n|} = \frac{k-1}{k}.$$

Remedies for Multiple Roots with Newton Method -1

1. **For a root of multiplicity *k*, restore quadratic convergence by modifying the formula to (if k is known)**

$$x_{n+1} = x_n - k\frac{f(x_n)}{f'(x_n)} \equiv g_k(x_n)$$

Why?

At $f(r) = 0$, $g_k(r) = r$. Based on

$f(x) = (x-r)^k Q(x)$, where $Q(r) \neq 0$,

we have

$$g'_k(x) = \frac{(r-x)\left\{k(r-x)QQ''+Q'\left[2kQ-(k-1)(r-x)Q'\right]\right\}}{\left[(r-x)Q'+kQ\right]^2}$$

We can easily see that $g'_k(r) = 0$, so the modified Newton method converge quadratically at multiple roots (including simple root where $k = 1$).

Remedies for Multiple Roots with Newton Method -2

With modified Newton method:

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

The third iterate is

$$x_3 = 1.00088 \text{ with } f(x_3) = 0.00000$$

Note: we also find that

$$e_{n+1} = 0.24 e_n^2,$$

confirming quadratic convergence.

Remedies for Multiple Roots with Newton Method -3

- But k is unknown in advance!!
- Guess a k by comparing a graph of f(x) with the plots of $(x-r)^k$ using an approximate r and various values of k.
  - The flatness will be similar, but this is not justified
- Divide f(x) by (x-r) and deflate the function, reducing the multiplicity by one.
    - But r is unknown
      - Dividing f by (x-s), where s is an approximate of r, does almost the same thing.

Remedies for Multiple Roots with Newton Method -4

2. If k is known

- **k=2**
  - Newton method can be applied to $f'(x)=0$ to converge quadratically to a double root of $f(x)=0$. **(simple root of $f'(x)=0$)**
- **k=3**
  - Similarly, the method can be applied to $f''(x)=0$ to get quadratic convergence to a triple root. **(simple root of $f''(x)=0$)**

$$f(x)=(x-r)^2Q(x),\ \text{where}\ Q(r)\neq 0,$$

$$f'(x)=2(x-r)Q(x)+(x-r)^2Q'(x)$$

$$=(x-r)[2Q(x)+(x-r)Q'(x)]$$

$$\text{where}\ 2Q(r)+(r-r)Q'(x)=2Q(r)\neq 0$$

Remedies for Multiple Roots with Newton Method -5

3. If k is known [Acton 1970]

A most tempting scheme:

- When f(x) has a root r of multiplicity *k*, we have

$$f(x) = (x-r)^k Q(x) \text{ and } Q(r) \neq 0$$

$$f'(x) = k(x-r)^{k-1}Q(x) + (x-r)^k Q'(x)$$

$$= (x-r)^{k-1}[kQ(x) + (x-r)Q'(x)]$$

- If we divide f(x) by f'(x), we effectively deflate f(x) n-1 times and we now work with a new function that has only a single root at x=r. Why? See next page.

Remedies for Multiple Roots with Newton Method -6

If $f(x)$ has a root of multiplici ty k at $x = r$,

$f(x) = (x-r)^k Q(x)$, where $Q(r) \neq 0$.

Let

$$S(x) = \frac{f(x)}{f'(x)} = \frac{(x-r)^k Q(x)}{k(x-r)^{k-1}Q(x) + (x-r)^k Q'(x)}$$

$$= (x-r)\frac{Q(x)}{kQ(x) + (x-r)Q'(x)}$$

which has a simple root at $x = r$ (since $Q(r) \neq 0$).

When $S(x)$ used in Newton formula, we have

$$x_{n+1} = x_n - \frac{S(x_n)}{S'(x_n)}$$

$$= x_n - \frac{f(x_n)f'(x_n)}{\left[f'(x_n)\right]^2 - f(x_n)f''(x_n)} \equiv g(x_n)$$

Accelerating convergence Aitken acceleration -1

- **Used to speed up convergence of any sequence that is linearly convergent.**

Definitions:

Given the sequence $\{p_n\}_{n=0}^{\infty}$, define the forward difference

$$\Delta p_n = p_{n+1} - p_n, \ \text{for } n \ge 0.$$

Higher powers $\Delta^k p_n$ is defined recursively by

$$\Delta^k p_n = \Delta^{k-1}(\Delta p_n), \ \text{for } n \ge 2.$$

Accelerating convergence Aitken acceleration -2

Theorem:

[From Friedman/Kandel, p90]

Assume that the sequence $\{p_n\}_{n=0}^{\infty}$ converge linearly to p and that $p_n - p \neq 0$ for all $n \geq 0$.

If there exists a real number A with $|A| < 1$ such that

$$\lim_{n\to\infty} \frac{p_{n+1} - p}{p_n - p} = A,$$

then the sequence $\{q_n\}_{n=0}^{\infty}$ defined by

$$q_n = p_n - \frac{(\Delta p_n)^2}{\Delta^2 p_n} = p_n - \frac{(p_{n+1} - p_n)^2}{p_{n+2} - 2p_{n+1} + p_n}$$

converges to p faster than $\{p_n\}_{n=0}^{\infty}$ in the sense that

$$\lim_{n\to\infty} \left| \frac{q_n - p}{p_n - p} \right| = 0.$$

Accelerating convergence Aitken acceleration -3

Proof :

Since there exists a real number A with $|A| < 1$ such that

$$\lim_{n\to\infty} \frac{p_{n+1} - p}{p_n - p} = A,$$

we have

$$\frac{p_{n+1} - p}{p_n - p} \approx A \approx \frac{p_{n+2} - p}{p_{n+1} - p}$$

when n is large.

This implies

$$(p_{n+1} - p)^2 \approx (p_n - p)(p_{n+2} - p)$$

Expanding the terms and cancelling p^2 yields

$$p \approx \frac{p_{n+2} p_n - p_{n+1}^2}{p_{n+2} - 2p_{n+1} + p_n}$$

$$= p_n - \frac{(p_{n+1} - p_n)^2}{p_{n+2} - 2p_{n+1} + p_n} = q_n.$$

We need to prove that $\{q_n\}_{n=0}^{\infty}$ converges to p faster than $\{p_n\}_{n=0}^{\infty}$ in the sense that

$$\lim_{n\to\infty} \left| \frac{q_n - p}{p_n - p} \right| = 0.$$

Accelerating convergence Aitken acceleration -4

Proof : (continued)

Let $e'_n = q_n - p$, then

$$e'_n = p_n - p - \frac{(p_{n+1} - p_n)^2}{p_{n+2} - 2p_{n+1} + p_n}$$

$$= e_n - \frac{(e_{n+1} - e_n)^2}{e_{n+2} - 2e_{n+1} + e_n}$$

$$= \frac{e_n e_{n+2} - e_{n+1}^2}{e_{n+2} - 2e_{n+1} + e_n}$$

Note that

Based on $\lim_{n\to\infty} \frac{e_{n+1}}{e_n} = A$,

$$e_{n+1} = (A + \theta_n)e_n$$

$$e_{n+2} = (A + \theta_{n+1})e_{n+1}$$

$$= (A + \theta_{n+1})(A + \theta_n)e_n$$

where $\theta_n, \theta_{n+1} \to 0$

as $n \to \infty$.

Accelerating convergence Aitken acceleration -5

Proof : (continued)

Therefore

$$
\begin{aligned}
e'_n
&= \frac{(A+\theta_{n+1})(A+\theta_n)e_n^2-(A+\theta_n)^2 e_n^2}{(A+\theta_{n+1})(A+\theta_n)e_n-2(A+\theta_n)e_n+e_n} \\
&= \frac{(A+\theta_{n+1})(A+\theta_n)-(A+\theta_n)^2}{(A+\theta_{n+1})(A+\theta_n)-2(A+\theta_n)+1}e_n \\
&= \frac{(A+\theta_n)[(A+\theta_{n+1})-(A+\theta_n)]}{(A^2-2A+1)+A\theta_{n+1}+A\theta_n+\theta_{n+1}\theta_n-2\theta_n} \\
&= \frac{(A+\theta_n)}{(A-1)^2+A(\theta_{n+1}+\theta_n)+\theta_n(\theta_{n+1}-2)}(\theta_{n+1}-\theta_n)\,e_n
\end{aligned}
$$

Hence

$$\frac{e'_n}{e_n}=\frac{(A+\theta_n)}{(A-1)^2+A(\theta_{n+1}+\theta_n)+\theta_n(\theta_{n+1}-2)}(\theta_{n+1}-\theta_n)$$

and

$$\lim_{n\to\infty}\left|\frac{e'_n}{e_n}\right|=\frac{A}{(A-1)^2}\lim_{n\to\infty}(\theta_{n+1}-\theta_n)=0.$$

Accelerating convergence Aitken acceleration -6

Advantages:

- **No significant additional computing time, because the time for computing q_n is negligible, once p_n, p_{n+1}, p_{n+2} are already given.**
- **Aitken acceleration speeds up the convergence for any sequence that is linearly convergent.**

Rate of convergence of Aitken method

– **Quadratic? NO!! Still linear, but faster than that for original sequence. WHY??**

Accelerating convergence Aitken acceleration -7

Theorem:

Consider $p_{n+1} = g(p_n)$. If the sequence $\{p_n\}_{n=0}^{\infty}$ converge linearly to p and

$$\lim_{n\to\infty} \frac{e_{n+1}}{e_n} = A \qquad (= g'(p)),$$

for $|A| < 1$, then the Aitken sequence $\{q_n\}_{n=0}^{\infty}$ behaves asymptotically according to

$$\lim_{n\to\infty} \frac{e'_{n+1}}{e'_n} = A^2 < A$$

Accelerating convergence Aitken acceleration -7

Proof : Since

$$e'_n = \frac{(A+\theta_{n+1})(A+\theta_n)e_n^2 - (A+\theta_n)^2 e_n^2}{(A+\theta_{n+1})(A+\theta_n)e_n - 2(A+\theta_n)e_n + e_n}$$

$$= \frac{(A+\theta_n)}{(A-1)^2 + A(\theta_{n+1}+\theta_n) + \theta_n(\theta_{n+1}-2)}(\theta_{n+1}-\theta_n)e_n$$

Hence

$$\frac{e'_{n+1}}{e'_n} = \frac{(A+\theta_{n+1})[(A-1)^2 + A(\theta_n+\theta_{n+1}) + \theta_n(\theta_{n+1}-2)]}{(A+\theta_n)[(A-1)^2 + A(\theta_{n+1}+\theta_{n+2}) + \theta_{n+1}(\theta_{n+2}-2)]}\frac{e_{n+1}(\theta_{n+2}-\theta_{n+1})}{e_n(\theta_{n+1}-\theta_n)}$$

Since

$$\lim_{n\to\infty}\theta_n = 0 \text{ and } \lim_{n\to\infty}\frac{e_{n+1}}{e_n} = A$$

We have

$$\lim_{n\to\infty}\frac{e'_{n+1}}{e'_n} = A\lim_{n\to\infty}\frac{(\theta_{n+2}-\theta_{n+1})}{(\theta_{n+1}-\theta_n)}.$$

We need to show that

$$\lim_{n\to\infty}\frac{(\theta_{n+2}-\theta_{n+1})}{(\theta_{n+1}-\theta_n)} = A.$$

Accelerating convergence Aitken acceleration -7

Proof :

Consider

$$g(x) = g(r) + (x-r)g'(r) + \frac{(x-r)^2}{2} g''(\xi),$$

where ξ is between x and r.

$$e_{n+1} = x_{n+1} - r = g(x_n) - g(r)$$

$$= (x_n - r)g'(r) + \frac{(x_n - r)^2}{2} g''(\xi_n),$$

where ξ_n is between x_n and r, so $\lim_{n\to\infty} \xi_n = r$.

Due to the continuity of g'', we can write

$g''(\xi_n) = g''(r) + \theta_n', \lim_{n\to\infty} \theta_n' = 0.$

Hence

$$e_{n+1} = e_n A + \frac{e_n^{\,2}}{2}\left(A' + \theta_n'\right),$$

where $g'(r) = A, g''(r) = A'$

Because $e_{n+1} = (A + \theta_n)e_n$, we obtain

$$e_{n+1} = e_n A + \frac{e_n^{\,2}}{2}\left(A' + \theta_n'\right) = (A + \theta_n)e_n$$

and $\theta_n = \dfrac{e_n}{2}\left(A' + \theta_n'\right).$

Finally,

$$\lim_{n\to\infty} \frac{\theta_{n+1}}{\theta_n} = \lim_{n\to\infty} \frac{\frac{e_{n+1}}{2}\left(A' + \theta_{n+1}'\right)}{\frac{e_n}{2}\left(A' + \theta_n'\right)}$$

$$= \lim_{n\to\infty} \left(\frac{e_{n+1}}{e_n} \frac{A' + \theta_{n+1}'}{A' + \theta_n'} \right) = \lim_{n\to\infty} \frac{e_{n+1}}{e_n} = A.$$

Therefore

$$\lim_{n\to\infty} \frac{\theta_{n+2} - \theta_{n+1}}{\theta_{n+1} - \theta_n} = \lim_{n\to\infty} \frac{\frac{\theta_{n+2}}{\theta_{n+1}} - 1}{1 - \frac{\theta_n}{\theta_{n+1}}} = \frac{A-1}{1 - \frac{1}{A}} = A$$

Accelerating convergence Aitken acceleration -9

Theorem:

Given a tolerance $\varepsilon > 0$, let N, N' denote the number of iterations required for convergence using fixed point iteration and Aitken's iteration, respectively. Then

$$\lim_{\varepsilon \to 0} \frac{N'}{N} = \frac{1}{2}$$

Accelerating convergence Aitken acceleration -8

N=11, N'=5

$|e_4/e_3|=0.312 \sim |A|=g'(s)=(3/8)\, s^2=0.308$

$|e'_4/e'_3|=0.096 \sim A^2=0.095$

Example 3.3.4.
Let $f(x) = 1 - (x^3/8)$, $0 \le x \le 1$ (Fig. 3.3.1) and consider the equation $x = f(x)$, given a first approximation $x_0 = 0$ and a tolerance $\epsilon = 10^{-6}$. The exact solution computed to nine significant digits is $s = 0.906795303$. A comparison between the performances of the SIM and ATKN is given in Table 3.3.3.

SIM: Fixed point iteration

Table 3.3.3. $x = 1 - (x^3/8)$, $0 \le x \le 1$, $x_0 = 0$, $\epsilon = 10^{-6}$

n	x_n	x'_n	$\lvert\epsilon_n/\epsilon_{n-1}\rvert$	$\epsilon'_n/\epsilon'_{n-1}$
0	0.000000000	0.888888889		
1	1.000000000	0.906020558	0.103	0.043
2	0.875000000	0.906717286	0.341	0.101
3	0.916259766	0.906788044	0.298	0.093
4	0.903846331	0.906794608	0.312	0.096
⋮				
12	0.906796083			

Accelerating convergence Aitken acceleration -10

Example 3.3.1.

Consider $x = e^{-x}$, $1/2 \le x \le 2/3$, $x_0 = 0.5$. Table 3.3.1 contains the first eight iterations, using the SIM, compared with eight iterations based on Aitken's scheme.

Table 3.3.1. $x = e^{-x}$ (Aitken's Method)

n	x_n	x'_n
0	0.500000	0.567624
1	0.606531	0.567299
2	0.545239	0.567193
3	0.579703	0.567159
4	0.560065	0.567148
5	0.571172	0.567145
6	0.564863	0.567144
7	0.568438	0.567143
8	0.566409	
⋮		
22	0.567143	

We see that ATKN yields the first 6 digits of the exact solution after 8 iterations, compared with the 22 that are needed for the SIM (to provide the same accuracy). □

Example 3.3.2.

Accelerating convergence Aitken acceleration -11

Exact solution to 8 decimal digits: 0.73908513

ITERATION

Table 3.3.2. $x = \cos x$ (Aitken's Method)

n	x_n	x'_n
0	1.00000000	0.72801036
1	0.54030231	0.73366516
2	0.85755322	0.73690629
3	0.65428979	0.73805042
4	0.79348036	0.73863610
5	0.70136877	0.73887658
6	0.76395968	0.73899224
7	0.72210243	0.73904251
8	0.75041776	0.73906595
9	0.73140404	0.73907638
10	0.74423735	0.73908118
11	0.73560474	
⋮		
26	0.73909441	

To approximate r within error 10^-5:
Aitken method: requires 11 iterations
Fixed-point iteration: requires 25 iterations.

Nonlinear systems

- **Nonlinear system**

$$
\begin{aligned}
f_1(x_1, x_2, x_3, \ldots, x_n) &= 0 \\
f_2(x_1, x_2, x_3, \ldots, x_n) &= 0 \\
&\vdots \\
&\vdots \\
f_n(x_1, x_2, x_3, \ldots, x_n) &= 0
\end{aligned}
$$

- **2x2 system**

$$
\begin{aligned}
f(x, y) &= 0 \\
g(x, y) &= 0
\end{aligned}
$$

Solution set : Regarded as the intersections of two algebraic curves.

Nonlinear systems

- **Example**

$$\begin{cases} x^2 + y^2 = 4 \\ e^x + y = 0 \end{cases}$$

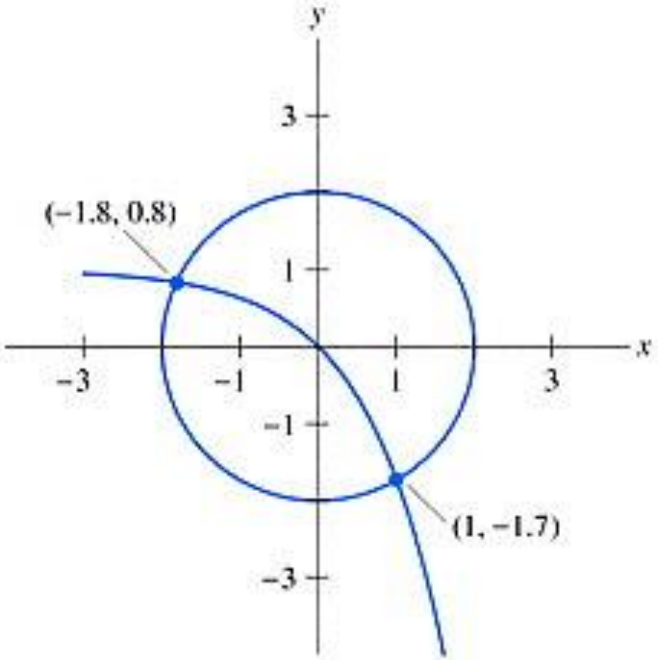


Figure 1.11

Nonlinear Systems Methods

Similar to solving f(x)=0

- **Fixed point iteration**
  - Different formulae behave differently
  - Converge linearly
- **Newton method**
  - Derivative vs. Jacobian matrix
  - Converge quadratically

Nonlinear Systems
Fixed Point Iteration

Consider the 2x2 system:

$$\begin{cases} f_1(x, y) = 0 \\ f_2(x, y) = 0 \end{cases}$$

Fixed point equation:

$$\begin{cases} x = g_1(x, y) \\ y = g_2(x, y) \end{cases}$$

If the starting point is sufficiently close to the fixed point (p, q), and if

$$\left|\frac{\partial g_1}{\partial x}(p,q)\right| + \left|\frac{\partial g_1}{\partial y}(p,q)\right| < 1 \text{ and}$$

$$\left|\frac{\partial g_2}{\partial x}(p,q)\right| + \left|\frac{\partial g_2}{\partial y}(p,q)\right| < 1$$

then the iteration converges to the fixed point.

Note:
If the conditions are not met, the iteration might diverge.

Nonlinear Systems Fixed Point Iteration

$$\begin{cases} x^2 - 2x - y + 0.5 = 0 \\ x^2 + 4y^2 - 4 = 0 \end{cases}$$

Fixed point formulation:

$$\begin{cases} x = \dfrac{x^2 - y + 0.5}{2} \\ y = \dfrac{-x^2 - 4y^2 + 8y + 4}{8} \end{cases}$$

Starting with (0,1), it converges to (-0.2,1.0).

Observe that

$$\left|\frac{\partial g_1}{\partial x}(p,q)\right| + \left|\frac{\partial g_1}{\partial y}(p,q)\right|$$

$$= |x| + |-0.5| < 1, \text{ and}$$

$$\left|\frac{\partial g_2}{\partial x}(p,q)\right| + \left|\frac{\partial g_2}{\partial y}(p,q)\right|$$

$$< \frac{|-x|}{4} + |-y+1| < 1$$

for $-0.5 < x < 0.5$ and $0.5 < y < 1.5$.

Starting with (2,0), it diverges away from the solution.

Nonlinear Systems
Newton Method

Newton method for solving $\begin{cases} f(x,y)=0 \\ g(x,y)=0 \end{cases}$

Let (r,s) be a root and expand both functions as a Taylor series about (x_i,y_i), where (x_i,y_i) is a point near the root:

$$\begin{cases} f(r,s)=0= f(x_i,y_i)+f_x(x_i,y_i)(r-x_i) \\ \qquad\qquad\qquad + f_y(x_i,y_i)(s-y_i)+\cdots \\ g(r,s)=0=g(x_i,y_i)+g_x(x_i,y_i)(r-x_i) \\ \qquad\qquad\qquad + g_y(x_i,y_i)(s-y_i)+\cdots \end{cases}$$

Truncating both series give

$$\begin{cases} 0= f(x_i,y_i)+f_x(x_i,y_i)(r-x_i)+f_y(x_i,y_i)(s-y_i) \\ 0=g(x_i,y_i)+g_x(x_i,y_i)(r-x_i)+g_y(x_i,y_i)(s-y_i) \end{cases}$$

Nonlinear systems Newton method

The system is rewritten as

$$\begin{cases} f_x(x_i, y_i)(r - x_i) + f_y(x_i, y_i)(s - y_i) = -f(x_i, y_i) \\ g_x(x_i, y_i)(r - x_i) + g_y(x_i, y_i)(s - y_i) = -g(x_i, y_i). \end{cases}$$

The iterate is derived by solving

$$\begin{cases} f_x(x_i, y_i)\Delta x_i + f_y(x_i, y_i)\Delta y_i = -f(x_i, y_i) \\ g_x(x_i, y_i)\Delta x_i + g_y(x_i, y_i)\Delta x_i = -g(x_i, y_i) \end{cases}$$

where $x_{i+1} = x_i + \Delta x_i$ and $y_{i+1} = y_i + \Delta y_i$ are improved estimate of the root.

Repeating this iteration until both $f(x_i)$ and $g(y_i)$ are close to zero.

Nonlinear Systems Newton Method

$$\begin{cases} f_x(x_i, y_i)\Delta x_i + f_y(x_i, y_i)\Delta y_i = -f(x_i, y_i) \\ g_x(x_i, y_i)\Delta x_i + g_y(x_i, y_i)\Delta x_i = -g(x_i, y_i) \end{cases}$$

can be rewritten as

$$J(x_i, y_i)\begin{bmatrix} \Delta x_i \\ \Delta y_i \end{bmatrix} = \begin{bmatrix} -f(x_i, y_i) \\ -g(x_i, y_i) \end{bmatrix}$$

If $J(x_i, y_i)$ is nonsingular, Δx_i and Δy_i can be found by solving the linear system.

New iterate is obtained by

$$\begin{bmatrix} x_{i+1} \\ y_{i+1} \end{bmatrix} = \begin{bmatrix} x_i \\ y_i \end{bmatrix} + \begin{bmatrix} \Delta x_i \\ \Delta y_i \end{bmatrix}.$$

Nonlinear Systems Newton Method

- **The Newton method for solving nonlinear system converges quadratically, but requiring**
  - **n^2+n function evaluations at each step**
    - **6 function evaluations for a 2x2 system**
    - **12 function evaluations for a 3x3 system**
  - **Solving an nxn linear system**