# Numerical Methods

## DS288 and UMC201

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# Fixed-Point Method

## Proof (C) Convergences

- Given that $\alpha$ is the fixed point of $g(\alpha) = \alpha$ and
- Further, $g(x) \in \mathbb{C}[a, b], \forall x \in [a, b]$ and $x_n = g(x_{n-1})$.
- Hence, for each $n \geq 1$,

$$\begin{aligned} |x_n - \alpha| &= |g(x_{n-1}) - g(\alpha)| = |g'(\zeta)(x_{n-1} - \alpha)| \\ &= |g'(\zeta)||x_{n-1} - \alpha| \qquad \text{from MVT} \\ &\leq k|x_{n-1} - \alpha| \qquad (1) \end{aligned}$$

- Inductively,

$$|x_n - \alpha| \leq k|x_{n-1} - \alpha| \leq \cdots \leq k^n|x_0 - \alpha|. \qquad (2)$$

- Since, $0 < k < 1, \implies \lim_{n\to\infty} k^n = 0$.
- Thus, $\lim_{n\to\infty}|x_n - \alpha| \leq \lim_{n\to\infty} k^n|x_0 - \alpha| = 0$. Hence, the sequence $\{x_n\}$ converges to the fixed point $\alpha$.

# Fixed-Point Method

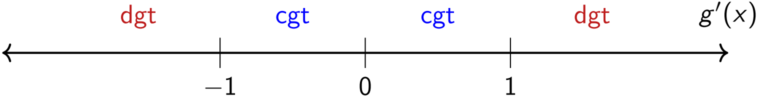
- Reformulate a equation to an equivalent fixed point problem:

$$f(x) = 0 \Leftrightarrow x = g(x) \tag{3}$$

- Use the iteration: with an initial guess $x_0$, compute a sequence

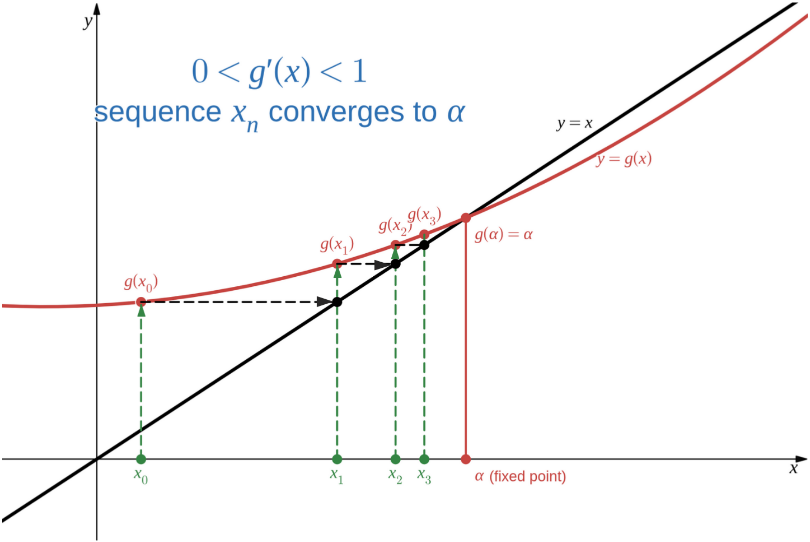
$$x_{n+1} = g(x_n), \;\; n \geq 0 \;\; \text{on the hope that} \;\; x_n \to \alpha$$

- Use the concept of a fixed point in a repeated manner to compute solution
- For solution, the graphs of $y = x$ and $y = g(x)$ must intersect




Case-I For $0 < g'(x) < 1$
Case-II For $-1 < g'(x) < 0$
Case-III For $g'(x) > 1$
Case-IV For $g'(x) < -1$

# Fixed-Point Method



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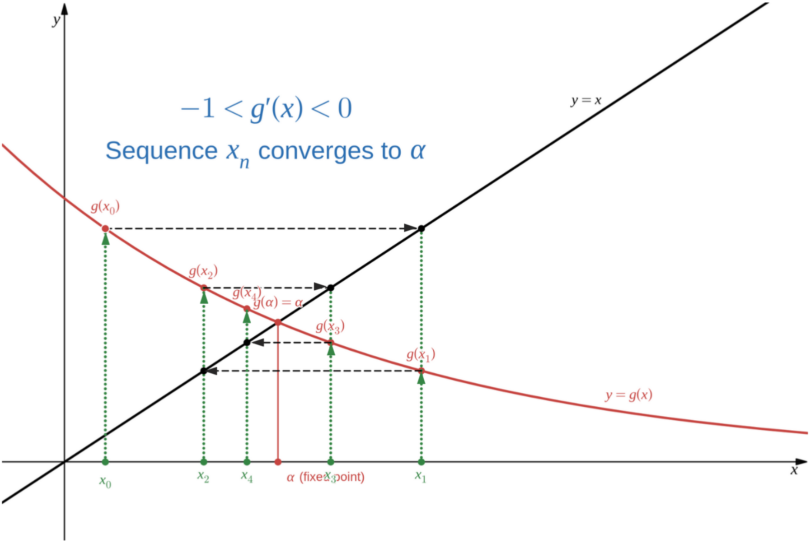

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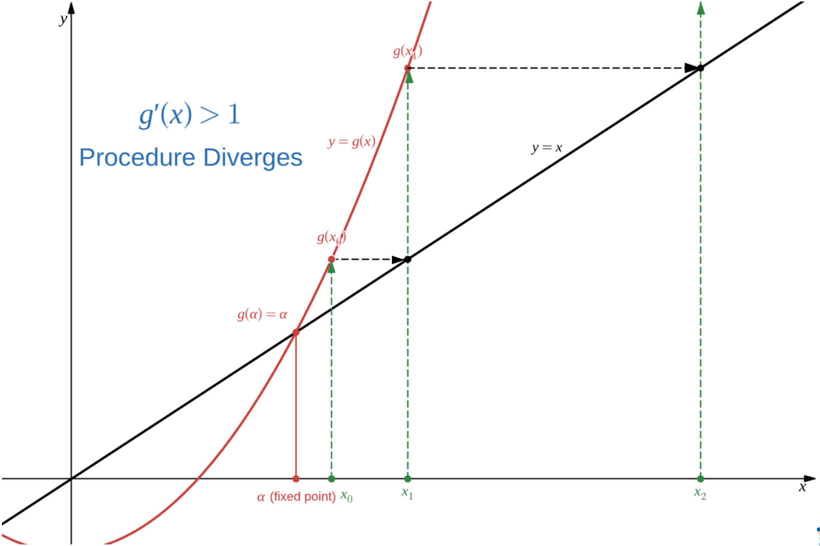

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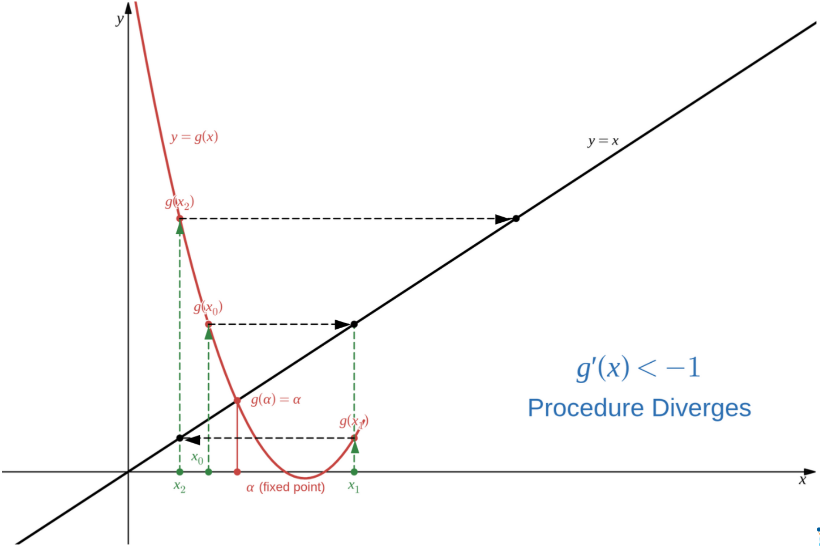
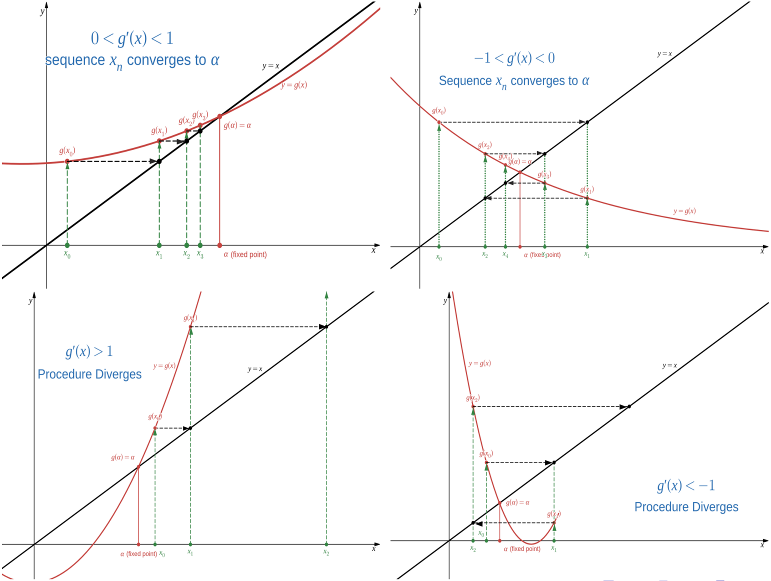



$g'(x) < -1$

Procedure Diverges

# Fixed-Point Method



# Error Estimation of Fixed-Point Method

- Since $|g'(x)| \leq k < 1$ for all $x \in I$: $\quad |e_{n+1}| = |g'(\xi_n)||e_n| \leq k|e_n|$
- induction: $\quad |e_{n+1}| \leq k|e_n| \leq k^2|e_{n-1}| \leq \cdots \leq k^{n+1}|e_0|$
- Therefore: $\quad |x_{n+1} - \alpha| \leq k^{n+1}|x_0 - \alpha|$

## Number of Iterations required for Fixed-Point Method

- To achieve an error tolerance $\epsilon > 0$, we need: $|x_n - \alpha| \leq k^n|x_0 - \alpha| < \epsilon$
- Taking logarithms: $n\ln(k) + \ln|x_0 - \alpha| < \ln(\epsilon)$
- Since $k < 1$, we have $\ln(k) < 0$, so:

$$n > \frac{\ln(\epsilon) - \ln|x_0 - \alpha|}{\ln(k)} = \frac{\ln\left(\frac{\epsilon}{|x_0-\alpha|}\right)}{\ln(k)}$$

- The minimum number of iterations required is: $N = \left\lceil \frac{\ln\left(\frac{\epsilon}{|x_0-\alpha|}\right)}{\ln(k)} \right\rceil$

# Order of Convergence

## Theorem

*Let $\alpha$ be a fixed point of $g(x)$. If $g'(\alpha) = 0$, $g''(\alpha) \neq 0$ and $g''$ is continuous with $|g''(x)| < M$ on an interval $I$ containing $\alpha$ Then*

(a) *There exists a $\delta > 0$ such that, for $x_0 \in [\alpha - \delta, \alpha + \delta]$, then $x_n = g(x_{n-1})$ converges quadratically to $\alpha$*

(b) $|x_{n+1} - \alpha| < \frac{M}{2}|x_n - \alpha|^2$, *for sufficiently large $n$*

## Taylor's Theorem

Suppose $f \in C^n[a, b]$, $f^{n+1}$ exists on $[a, b]$, and $x_0 \in [a, b]$. Then for every $x \in [a, b]$ there exists a number $\zeta$ in $x_0$ and $x$, such that

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \cdots \frac{f^n(x_0)}{n!}(x - x_0)^n + R_n(x)$$

$$\text{where} \quad R_n(x) = \frac{f^{n+1}(\zeta)}{(n+1)!}(x - x_0)^{n+1}$$

# Order of Convergence

## Proof (a)

- The Taylor polynomial of $g(x)$ for $x \in [\alpha - \delta, \alpha + \delta]$, where $\delta > 0$ and $[\alpha - \delta, \alpha + \delta] \subset I$

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

  where $\xi$ lies between $x$ and $\alpha$.
- Using $g(\alpha) = \alpha$ and $g'(\alpha) = 0$, we get

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

- Substituting $x = x_n$, $x_{n+1} = g(x_n) = \alpha + \frac{g''(\xi_n)}{2}(x_n - \alpha)^2$

$$|x_{n+1} - \alpha| = \frac{g''(\xi_n)}{2}|x_n - \alpha|^2$$

# Order of Convergence

## Proof (a) continues

- Since $|g'(x)| < k < 1$ and $g(x) \in [\alpha - \delta, \alpha + \delta], \forall x \in [\alpha - \delta, \alpha + \delta]$. And $\xi_n$ lies between $x_n$ and $\alpha$ for each $n$. Hence, $\{x_n\} \to \alpha$ and $\{\xi_n\} \to \alpha$, as $n \to \infty$. Therefore,

$$\lim_{n\to\infty} \frac{|x_{n+1} - \alpha|}{|x_n - \alpha|^2} = \frac{|g''(\alpha)|}{2}$$

Hence the sequence $x_n$ is quadratically convergent if $g''(\alpha) \neq 0$.

## Proof (b)

- Since $g''$ is continuous and $|g''(x)| < M$ on the interval $[\alpha - \delta, \alpha + \delta]$, therefore, for sufficiently large $n$

$$|x_{n+1} - \alpha| < \frac{M}{2}|x_n - \alpha|^2$$

# Order of Convergence

**Theorem**

If the iteration function $g(x)$ is such that

(I) $g^{(m)}(x)$ is continuous and bounded in some neighborhood of the fixed point $\alpha$.

(II) $g'(\alpha) = g'(\alpha) = \cdots g^{(m-1)}(\alpha) = 0,$ but $g^{(m)}(\alpha) \neq 0$.

Then the fixed point iteration $x_{n+1} = g(x_n)$ has order of convergence $m$.

## Special Cases for convergence

- Linear Convergence $(m = 1)$: When $g'(\alpha) \neq 0$
- Quadratic $(m = 2)$: When $g'(\alpha) = 0$ and $g''(\alpha) \neq 0$
- Cubic $(m = 3)$: When $g'(\alpha) = g''(\alpha) = 0$ and $g'''(\alpha) \neq 0$

Convergence rate improves as more derivatives vanish at the fixed point.

# Advantages and disadvantages

### Advantage

- Converges fast (if it converges) in comparison with Bisection method.
- Order of converges is two if $g'(\alpha) = 0$ and $g''(\alpha) \neq 0$. (Provided $g''(\alpha)$ continuous and bounded)

### Disadvantage

- If $g$ does not satisfies the required properties given in the convergence theorem then the method may or may not converge.

# Muller's Method

# Muller Method

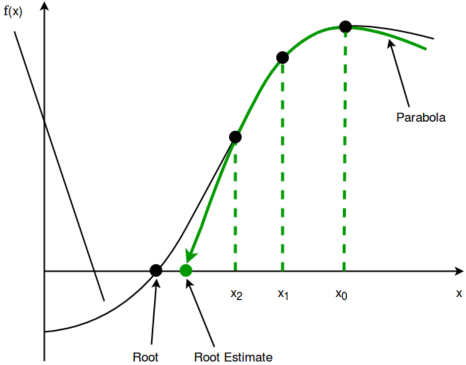
- Muller's method is an extension of the secant method.
- It starts with three given initial approximation (but the secant method starts with two given initial approximation)
- It used the quadratic polynomial (parabola) to find a root for the next approximation (but the straight line for the secant method)

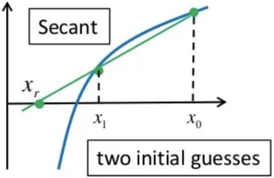
➢ Given $f(x) = 0$ with given initial guesses be $x_0, x_1$ and $x_2$

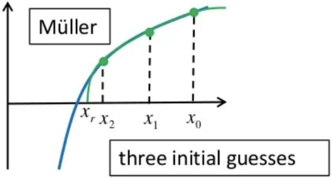
➢ The next approximation $x_3$ is determined by considering the intersection of the $X$-axis with the parabola through $(x_0, f(x_0)), (x_1, f(x_1)),$ and $(x_2, f(x_2))$.

➢ The parabola fit function facilitates finding both real and complex roots

# Muller Method



# Derivation of Muller's Method

- Define the parabola (quadratic polynomial) as

$$P(x) = a(x - x_2)^2 + b(x - x_2) + c$$

that passes through $(x_0, f(x_0)), (x_1, f(x_1))$, and $(x_2, f(x_2))$.

- We determine the coefficients $a, b$ and $c$ by evaluating $P(x)$ at the given three points, $x_0, x_1$ and $x_2$ .
- Using the conditions

$$\begin{aligned} f(x_0) &= a(x_0 - x_2)^2 + b(x_0 - x_2) + c \\ f(x_1) &= a(x_1 - x_2)^2 + b(x_1 - x_2) + c \\ f(x_2) &= a.0^2 + b.0 + c = c \end{aligned}$$

- Solving the first two equations, we get

# Derivation of Muller's Method

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

$$b = \frac{(x_0 - x_2)^2[f(x_1) - f(x_2)] - (x_1 - x_2)^2[f(x_0) - f(x_2)]}{(x_0 - x_2)(x_1 - x_2)(x_0 - x_1)}$$

$$c = f(x_2)$$

- After computing a, b and c, we solve the root of the equation

$$P(x) = a(x - x_2)^2 + b(x - x_2) + c = 0 :$$

- The solution of the equation

$$x - x_2 = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

- By rationalizing the numerator of R.H.S. of the above equation,

$$x = x_2 - \frac{2c}{b \pm \sqrt{b^2 - 4ac}}$$

# Muller Method

- This formula gives two possibilities for the next approximation $x = x_3$, depending on the sign of the radical term.
- The sign is chosen to agree with the sign of $b$. Hence, the denominator will be the largest (magnitude) and will result in $x_3$ being selected as the closest zero of $P(x)$ to $x_2$.
- The next approximation is given by

$$x_3 = x_2 - \frac{2c}{b + sgn(b)\sqrt{b^2 - 4ac}}$$

- where
$$\begin{aligned} sgn(b) &= +1 \quad \text{if } b > 0 \\ &= -1 \quad \text{if } b < 0 \end{aligned} \tag{4}$$

- Once $x_3$ is determined, the procedure reinitialized using $x_1, x_2, x_3$ in place of $x_0$, $x_1$, $x_2$ to determine $x_4$.

# Muller Method

- Since, there will be two roots, but we have to take that one which is closer to $x_2$. To avoid round-off errors due to subtraction of nearby equal numbers, use the following equation:

$$x_3 = x_2 - \frac{2c}{b + sgn(b)\sqrt{b^2 - 4ac}} \tag{5}$$

- where
$$\begin{aligned} sgn(b) &= +1 \quad \text{if } b > 0 \\ &= -1 \quad \text{if } b < 0 \end{aligned} \tag{6}$$

- Now, since, root of $p(x)$ has to be closer to $x_2$, so we have to take that value which has a greater denominator out of the two values possible from the above equation.

# Muller method for complex root

- Let $f : \mathbb{C} \to \mathbb{C}$ be a complex valued function. We begin by assuming $x_0, x_1, x_2 \in \mathbb{R}$.
- It is worth noticing the following case from the equation (5)
  (I) $x_0, x_1, x_2 \in \mathbb{R}$; but $x_3 \notin \mathbb{R}$ due to the presence of $\sqrt{b^2 - 4ac}$.
- This raises the question of what $sgn(b)$ means when $b \in \mathbb{C}$. In such a case, if $b = x_b + iy_b$, where $i$ is the imaginary unit.
- We define $sgn(b) = sgn(x_b)$. A drawback of this approach is that it does not account for the case when $b \in i\mathbb{R}$, i.e. when $b$ is purely imaginary.
- However, such cases seldom arise as the imaginary parts are often the result of numerical inaccuracies in calculation.

# Example

## Example

Find a root correct up to 3 decimal places of the equation $f(x) = 3x + \sin x - e^x$ between 0 and 1 by Muller's method.

- Consider $x_0 = 0, x_1 = 1$ and $x_2 = 0.5$.
- Thus, $f_2 = 0.330704, f_1 = 1.123189, f_0 = -1$.
- Now $a = 1.07644, b = 2.12319, c = 0.330704$.
- First approximation: $x_3 = 0.354914$
- Similarly, second approximation: $x_4 = 0.360465$.

  Hints : $a = 0.808314, b = 2.4980, c = 0.0138066$.
- Third approximation $x_4 = 0.3604217$
- Hence the solution correct up to 3 decimal digits is 0.3604217.

# Advantages and disadvantages

## Advantage

- Converges to a root faster (if it converges) than the Bisection, Secant, and Regula Falsi methods.
- The initial approximations need not bracket the root.
- Sometimes, fewer iterations needed in comparison with Newton's method
- Does not need the evaluation of derivatives.
- It is possible to approximate complex roots with a real initial approximation.
- Order of convergence of Muller's Method is **1.84.** (derivation is omitted)

## Disadvantage

- Sometimes, Muller's method diverges.
- Three good initial approximations of the root are needed.
- If the data points are very close or lie on a straight line, there are accuracy problems in computing the coefficients of the quadratic and more problems in determining its roots.
- Coding for Muller's method is more complicated than for other methods.

# Summary of Root Finding Methods

| Method | Root Type | Order of Convergence | Guarantee of Convergence |
|---|---|---|---|
| Bisection | simple | $\alpha = 1$ | Yes |
| | multiple (odd) | $\alpha = 1$ | Yes |
| | multiple (even) | Not Available | Not Available |
| False Position | simple | $\alpha = 1$ | Yes |
| | multiple (odd) | $\alpha = 1$ | Yes |
| | multiple (even) | Not Available | Not Available |
| Secant | simple | $\alpha = 1.62$ | No |
| | multiple | $\alpha = 1$ | No |
| Muller's Method | simple | $\alpha = 1.84$ | No |
| Newton's | simple | $\alpha = 2$ | No |
| | multiple | $\alpha = 1$ | No |
| Modified Newton's | simple | $\alpha = 2$ | No |
| | multiple | $\alpha = 2$ | No |


ANY
QUESTIONS?