
Numerical Methods

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Outline

- Introduction
- Approximations and Errors
- Roots of Equations
- Systems of linear algebraic equations
- Curve Fitting
- Numerical Differentiation and Integration

Roots of Equations

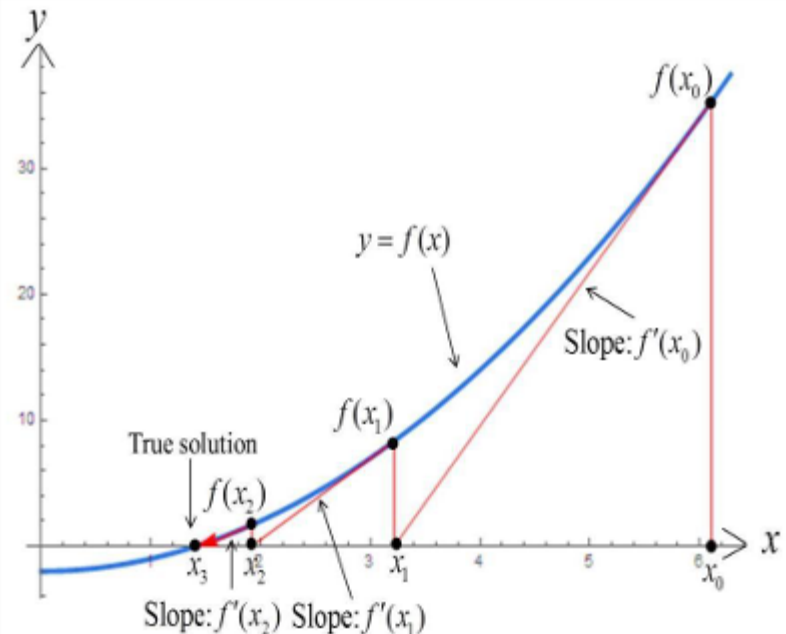
Open Methods

- The idea of this method is to consider at least one initial guess which is not necessarily bracket the root.
- Normally, the chosen initial value(s) must be close to the actual root that can be found by plotting the given function against its independent variable.
- In every step of root improvement, x_r of previous step is considered as the previous value for the present step.
- In general, open methods provides no guarantee of convergence to the true value, but once it is converge, it will converge faster than bracketing methods.



Newton-Raphson Method

- It is an open method for finding roots of $f(x) = 0$ by using the successive slope of the tangent line.
- The Newton Raphson method is applicable if $f(x)$ is continuous and differentiable.
- **Figure 6** shows the graphical illustration of Newton Raphson method
- Numerical scheme starts by choosing the initial point, x_0 as the first estimation of the solution.
- The improvement of the estimation of x_1 is obtained by taking the tangent line to $f(x)$ at the point $(x_0, f(x_0))$ and extrapolate the tangent line to find the point of intersection with an x -axis.



Newton-Raphson Method

Algorithm

For the continuous and differentiable function, $f(x) = 0$:

Step 1: Choose initial value, x_0 and find $f'(x_0)$.

Step 2: Compute the next estimate, x_{i+1} by using Newton Raphson formula

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

Step 3: Calculate the approximate percent relative error, ε_a

$$\varepsilon_a = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| \times 100\%$$

Step 4: Compare ε_s with ε_a . If $\varepsilon_a < \varepsilon_s$, the computation is stopped. Otherwise, repeat **Step 2**.

Newton-Raphson Method

Find the real root of the equation using Newton-Raphson's Method

$$f(x) = x^3 + 4x^2 - 1 = 0, \quad f'(x) = 3x^2 + 4 \cdot 2x - 0$$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{x_n^3 + 4x_n^2 - 1}{3x_n^2 + 8x_n}$$

x_0	0.5
x_1	0.473684211
x_2	0.472834787
x_3	0.472833909
x_4	0.472833909

Newton-Raphson Method

- The Newton-Raphson method requires the calculation of the *derivative* of a function, which is *not always easy*.
- If f' *vanishes* at an iteration point, then the method will *fail to converge*.
- When the step is *too large* or the value is *oscillating*, other more conservative methods should take over the case.

Secant Method

- In many cases, the derivative of a function is very difficult to find or even is not differentiable.
- Alternative approach is by using secant method.

- The slope in Newton's Rapshon method is substituted with backward finite divided difference

$$f'(x_i) = \frac{f(x_{i-1}) - f(x_i)}{x_{i-1} - x_i}$$

- The secant method formula is:

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

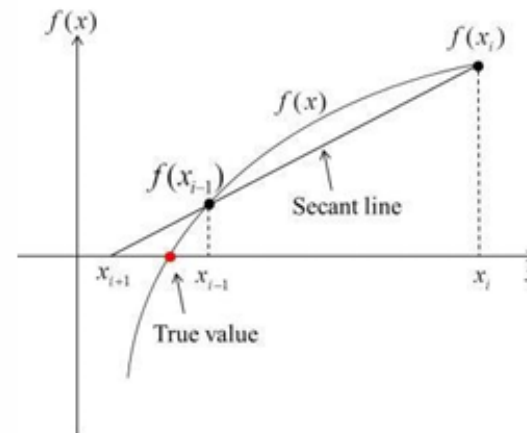


Figure 7: Graphical Illustration of Secant Method

Secant Method

Algorithm

For the continuous function, $f(x) = 0$:

Step 1: Choose initial values, x_{-1} and x_0 . Find $f(x_{-1})$ and $f(x_0)$.

Step 2: Compute the next estimate, x_{i+1} by using secant method formula

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

Step 3: Calculate the approximate percent relative error, ε_a

$$\varepsilon_a = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| \times 100\%$$

Step 4: Compare ε_s with ε_a . If $\varepsilon_a < \varepsilon_s$, the computation is stopped. Otherwise, repeat **Step 2**.

Secant Method

Example 9

Determine one of the real root(s) of $f(x) = -12 - 21x + 18x^2 - 2.4x^3$ by using secant method with initial guesses of $x_{-1} = 1.0$ and $x_0 = 1.3$. Perform the computation until $\varepsilon_a < 5\%$.

Solution

First iteration, $x_{-1} = 1.0$ and $x_0 = 1.3$

$$f(1.0) = -17.4$$

$$f(1.3) = -14.528$$

$$\begin{aligned}x_1 &= x_0 - \left[\frac{f(x_0)(x_{-1} - x_0)}{f(x_{-1}) - f(x_0)} \right] \\&= 1.3 - \left[\frac{-14.528(1 - 1.3)}{-17.4 + 14.528} \right] = 2.6075\end{aligned}$$

$$\varepsilon_a = \left| \frac{2.6075 - 1.3}{2.6075} \right| \times 100\% = 50.14\% > \varepsilon_s$$

Secant Method

Continue the second iteration and the results are summarised as follows.

No. of Iteration	i	x_{i-1}	x_i	$f(x_{i-1})$	$f(x_i)$	x_{i+1}	$\varepsilon_a(\%)$
1	0	1	1.3	-17.4	-14.1527	2.6075	50.14
2	1	1.3	2.6075	-14.1528	13.0780	1.9796	31.72
3	2	2.6075	1.9796	13.0780	-1.6519	2.0500	3.44

Therefore, after three iterations the approximated root of $f(x)$ is $x_3 = 2.0500$ with $\varepsilon_a = 3.44\%$.

Advantages of Secant Method

1. It converges at faster than a linear rate, so that it is more rapidly convergent than the bisection method.
2. It does not require use of the derivative of the function, something that is not available in a number of applications.
3. It requires only one function evaluation per iteration, as compared with Newton's method which requires two.

Disadvantages of Secant Method

1. It may not converge.
2. There is no guaranteed error bound for the computed iterates.
3. It is likely to have difficulty if $f'(\alpha) = 0$. This means the x-axis is tangent to the graph of $y = f(x)$ at $x = \alpha$.
4. Newton's method generalizes more easily to new methods for solving simultaneous systems of nonlinear equations.

Summary

Method	Advantages	Disadvantages
Bisection	<ul style="list-style-type: none">- Easy, Reliable, Convergent- One function evaluation per iteration- No knowledge of derivative is needed	<ul style="list-style-type: none">- Slow- Needs an interval $[a,b]$ containing the root, i.e., $f(a)f(b) < 0$
Newton	<ul style="list-style-type: none">- Fast (if near the root)- Two function evaluations per iteration	<ul style="list-style-type: none">- May diverge- Needs derivative and an initial guess x_0 such that $f'(x_0)$ is nonzero
Secant	<ul style="list-style-type: none">- Fast (slower than Newton)- One function evaluation per iteration- No knowledge of derivative is needed	<ul style="list-style-type: none">- May diverge- Needs two initial points guess x_0, x_1 such that $f(x_0) - f(x_1)$ is nonzero