

Numerical methods: root finding techniques

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Introduction i

The roots or zeros of a function $f(x)$ are the values x such that

$$f(x) = 0$$

or equivalently, finding the roots of $f(x) - g(x) = 0$ is the same as solving the equation

$$f(x) = g(x)$$

For example, the equation of state of real gases can be approximated by the van der Waals equation:

$$\left(p + \frac{an^2}{V^2} \right) \left(\frac{V}{n} - b \right) = RT$$

finding the volume for a range of temperatures, pressures, and number of moles requires a root finding algorithm.

Many root finding algorithms exist and most are iterative schemes, that is, they approach the "solution" by subsequent improved approximations.

- Bracketing methods
 - Bisection method
 - False-position method
 - ...
- Open methods
 - Newton-Raphson method
 - Secant method
 - ...

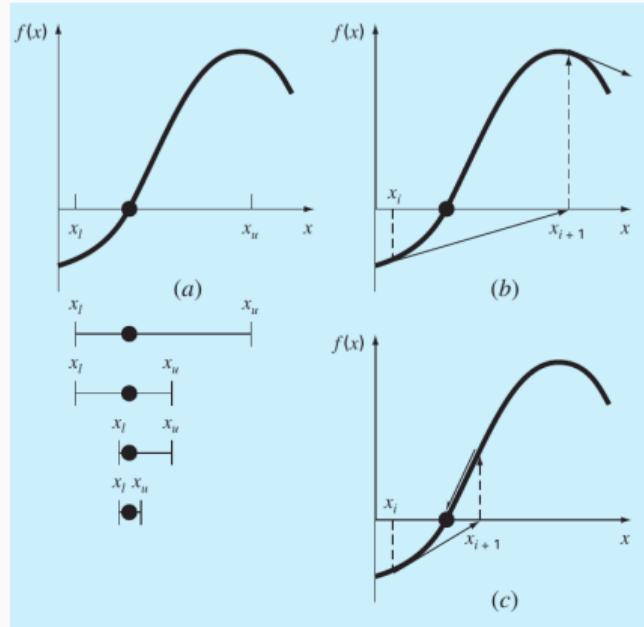


Figure 1: Comparison of bisection and open methods

Bisection method i

The bisection method starts with an interval $[a, b]$ (i.e. two guesses). If the function is continuous and $f(a)f(b) < 0$ then the root can be found, but it may be slow to get there...

The algorithm proceeds

- by cutting in half the size of the interval and
- finding which sub-interval satisfies $f(x_1)f(x_2) < 0$.
- The procedure (cut and check) is repeated until the error is "small enough!". The numerical root is the mid-point of the last interval

Exercise

Use the bisection method to find the root of the function

$$f(x) = \frac{1}{2} - e^{-x}$$

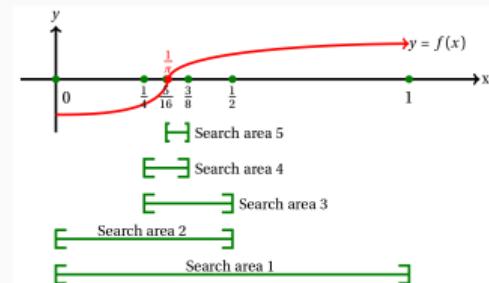


Figure 2: The bisection method

False-position method

The bisection is a "brute-force" method that does not take into account the properties of the function it is trying to find the roots of.

The *regula falsi* or false-position or linear interpolation method uses the relative values of the function at the end points to find an improved estimate of the root, which is given by:

$$x_r = x_u - \frac{f(x_u)(x_l - x_u)}{f(x_l) - f(x_u)}$$

→ the new sub-interval, either $[x_l, x_r]$ or $[x_r, x_u]$, is chosen as in the bisection method.

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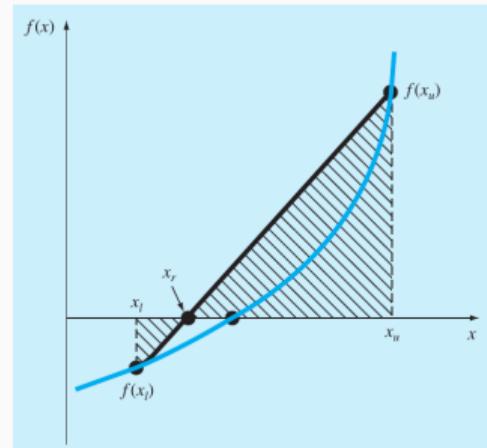


Figure 3: The regula falsi method

Newton-Raphson Method

This is one of the most widely used root finding algorithms. It requires:

- one initial guess value for the root
- the first derivative of the function

The improved estimate of the root is given by:

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

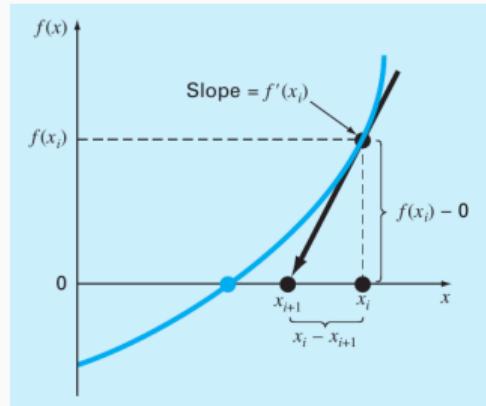


Figure 4: Newton-Raphson method

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But in some cases it can fail!

Backtracking is a technique to stop the search of the zero and change the guess value.

If a new guess $x_i + \delta x$, where $\delta x = -f(x)/f'(x)$, increases the magnitude of the function

$$|f(x_i + \delta x)| > |f(x_i)|$$

then we go back to x_i and decrease the size of δx by a factor α and keep doing it until

$$|f(x_i + \delta x)| < |f(x_i)|$$

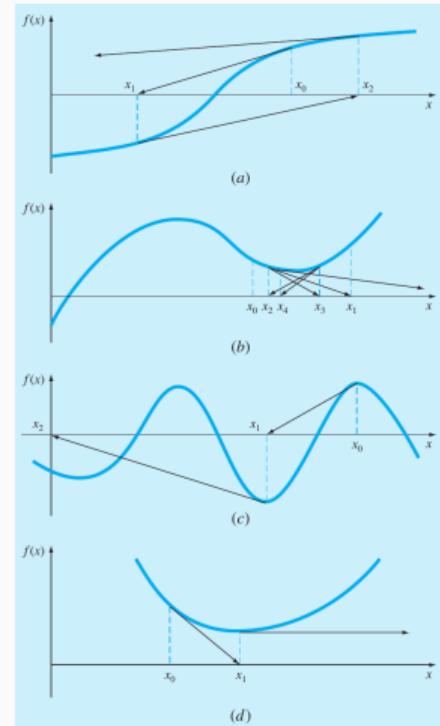


Figure 4: Examples of poor convergence of the Newton-Raphson method

The Secant Method

The secant method uses the numerically evaluated derivative. This is needed when the analytical expression of the derivative of the function $f(x)$ is not known or easily evaluated.

In the secant method the derivative is approximated as a *backward finite divided difference*:

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

The iterative equation for the improved estimate of the root is then given by:

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

This approach requires two initial estimates of x

→ the secant method and the false position method are similar, but different in important ways.

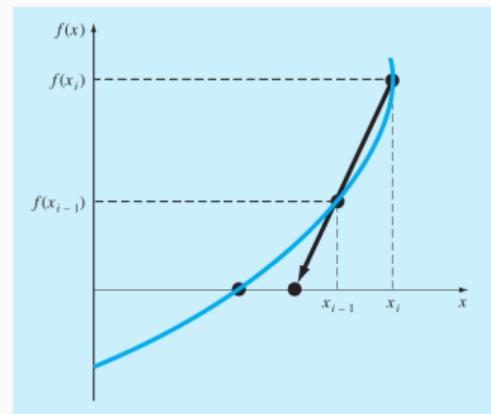


Figure 5: The secant method

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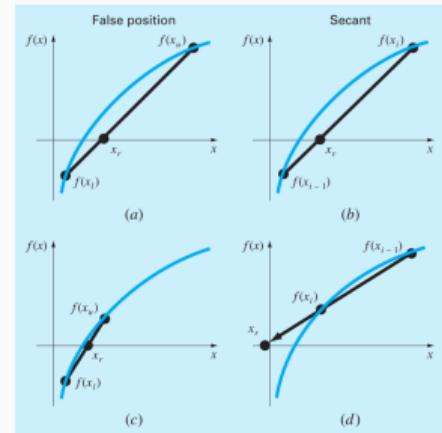


Figure 5: Comparison of the false position and secant methods

The modified Secant Method

Instead of using two values to estimate the initial derivative, we can use a small perturbation δx_i to calculate the derivative. In this case the iterative equation is:

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

Exercise

Use the open methods discussed (Newton-Raphson, secant and modified secant) to find the root of the function

$$f(x) = \frac{1}{2} - e^{-x}$$

- compare the various methods (speed, number of iterations, accuracy, ...) and discuss your results