

## Numerical methods: root finding techniques

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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

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

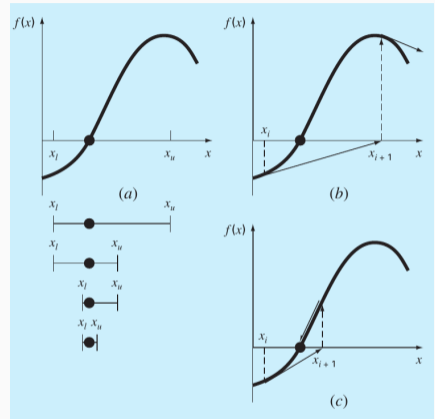
For example, the equation of state of real gases can be approximated by the van der Waals equation:

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

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

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

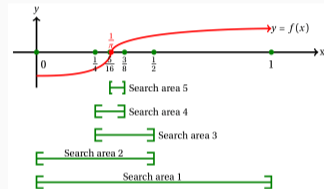


Figure 2: The bisection method

# 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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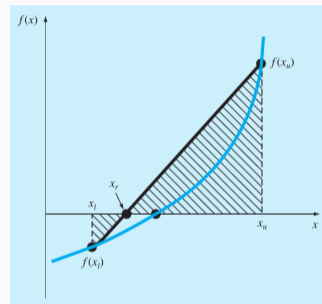


Figure 3: The regula falsi method

# 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:

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

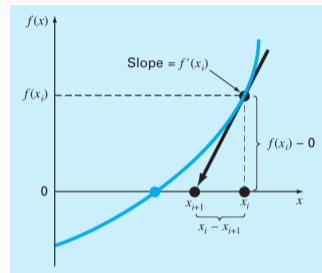


Figure 4: Newton-Raphson method

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But in some cases it can fail!

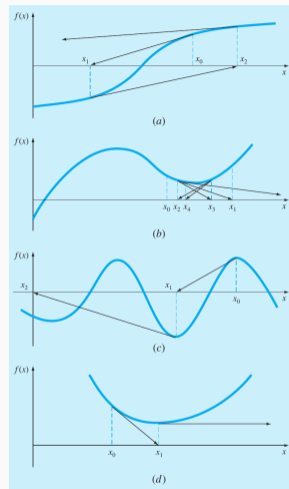
**Backtracking** is a technique to stop the search of the zero and change the guess value.

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  $\delta x$  by a factor  $\alpha$  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.

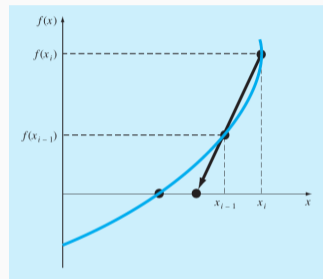


Figure 5: The secant method

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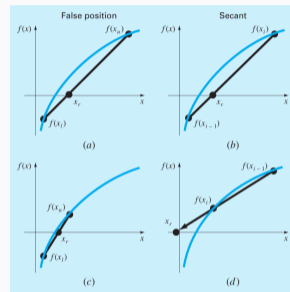
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**Figure 5:** Comparison of the false position and secant methods

Instead of using two values to estimate the initial derivative, we can use a small perturbation  $\delta x_i$  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