Finding roots of nonlinear equations

From Press et al. **Numerical Recipes**, Chapter 9

Easy and hard cases

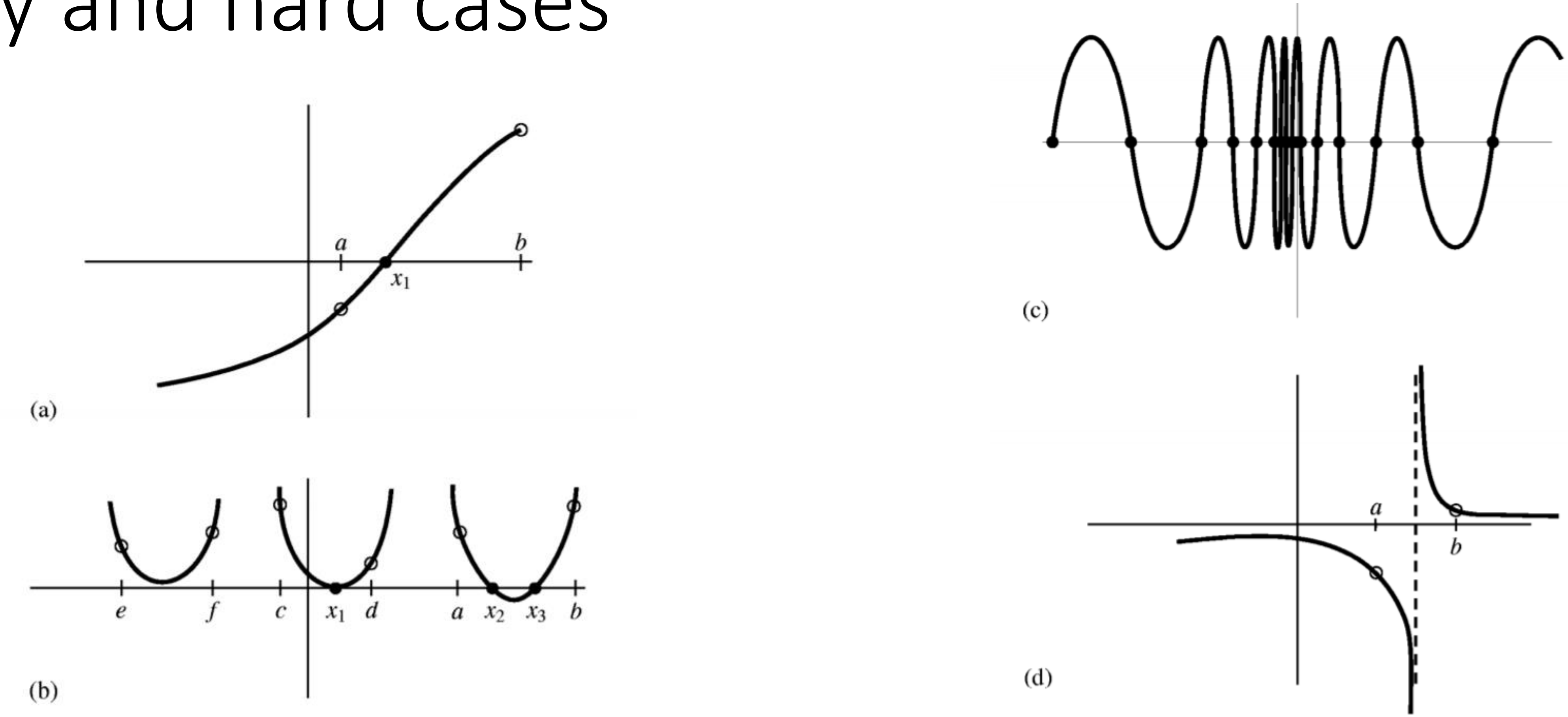
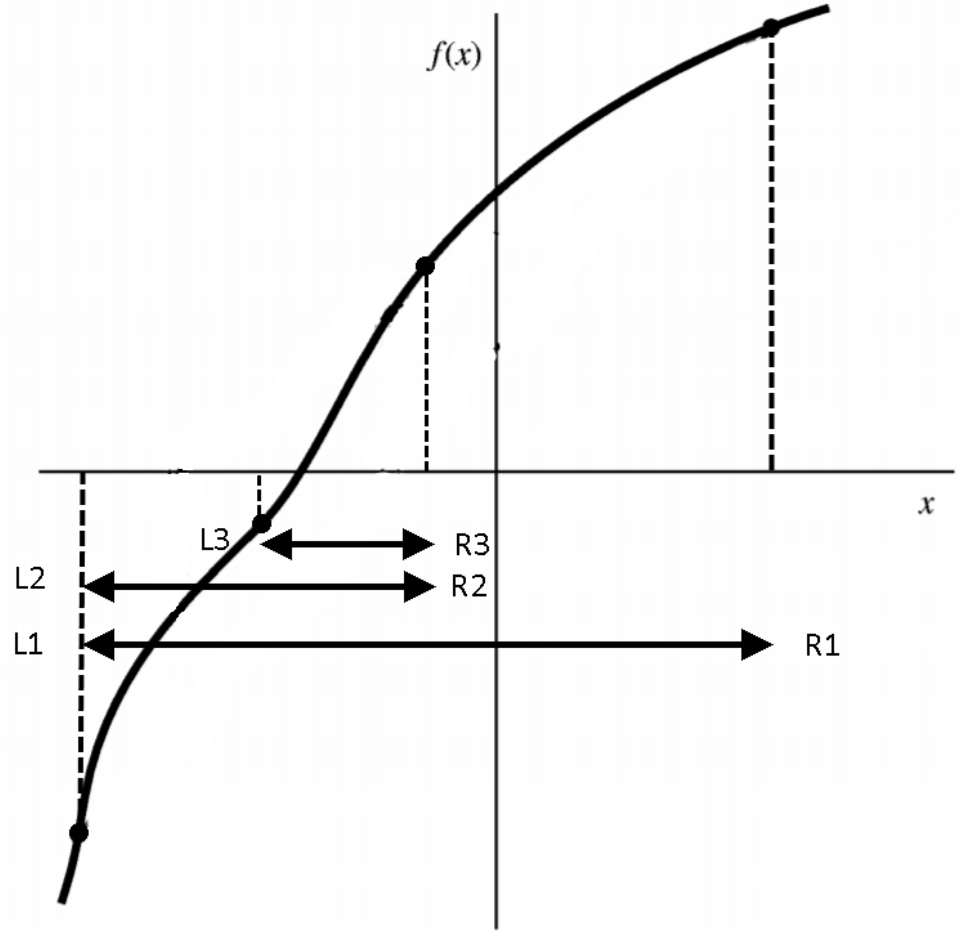


Figure 9.1.1. Some situations encountered while root finding: (a) shows an isolated root x_1 bracketed by two points a and b at which the function has opposite signs; (b) illustrates that there is not necessarily a sign change in the function near a double root (in fact, there is not necessarily a root!); (c) is a pathological function with many roots; in (d) the function has opposite signs at points a and b, but the points bracket a singularity, not a root.

Bisection method



Evaluate the function at the interval's midpoint and examine its sign. Use the midpoint to replace whichever limit has the same sign. After each iteration the bounds containing the root decrease by a factor of two. If after n iterations the root is known to be within an interval of size ϵ_n, then after the next iteration it will be bracketed within an interval of size

$$\epsilon_{n+1} = \epsilon_n/2 \qquad (9.1.2)$$

Secant method

- Not bracketed

$$\lim_{k \to \infty} |\epsilon_{k+1}| \approx \text{const} \times |\epsilon_k|^{1.618}$$

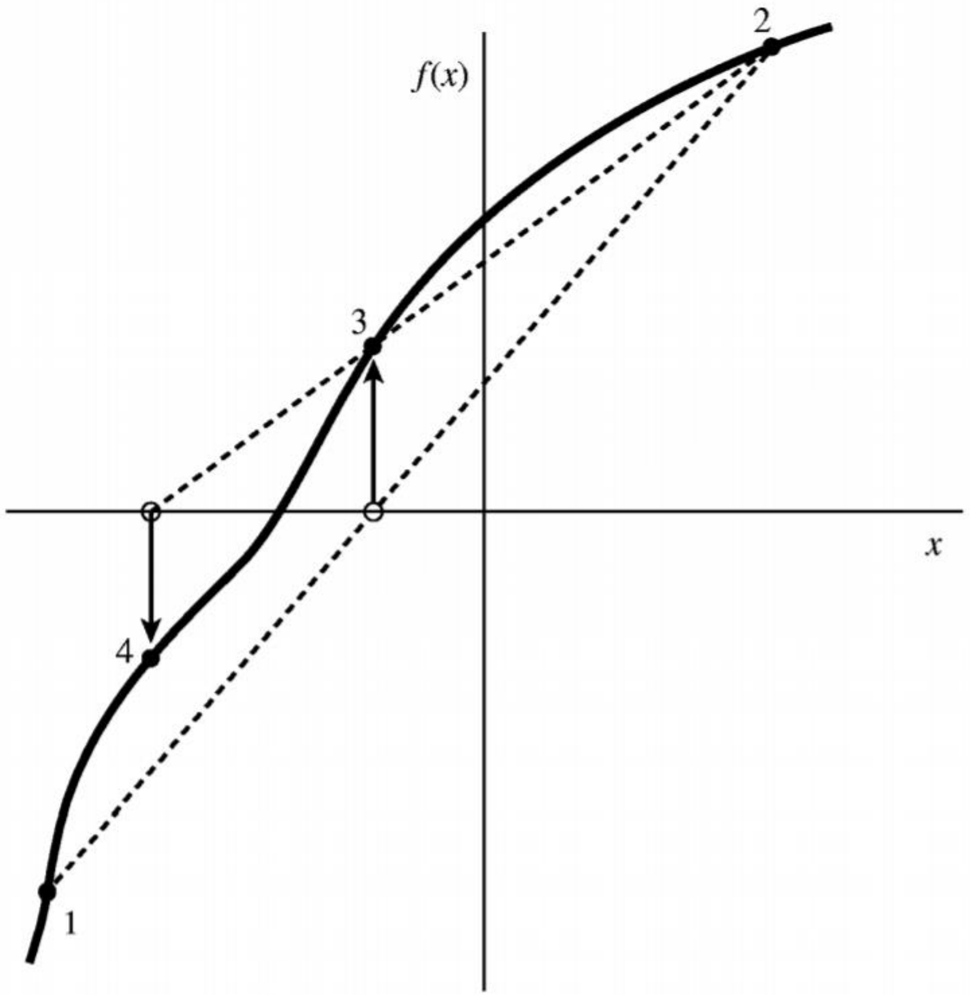


Figure 9.2.1. Secant method. Extrapolation or interpolation lines (dashed) are drawn through the two most recently evaluated points, whether or not they bracket the function. The points are numbered in the order that they are used.

False position method ("Regula falsi")

- Bracketed

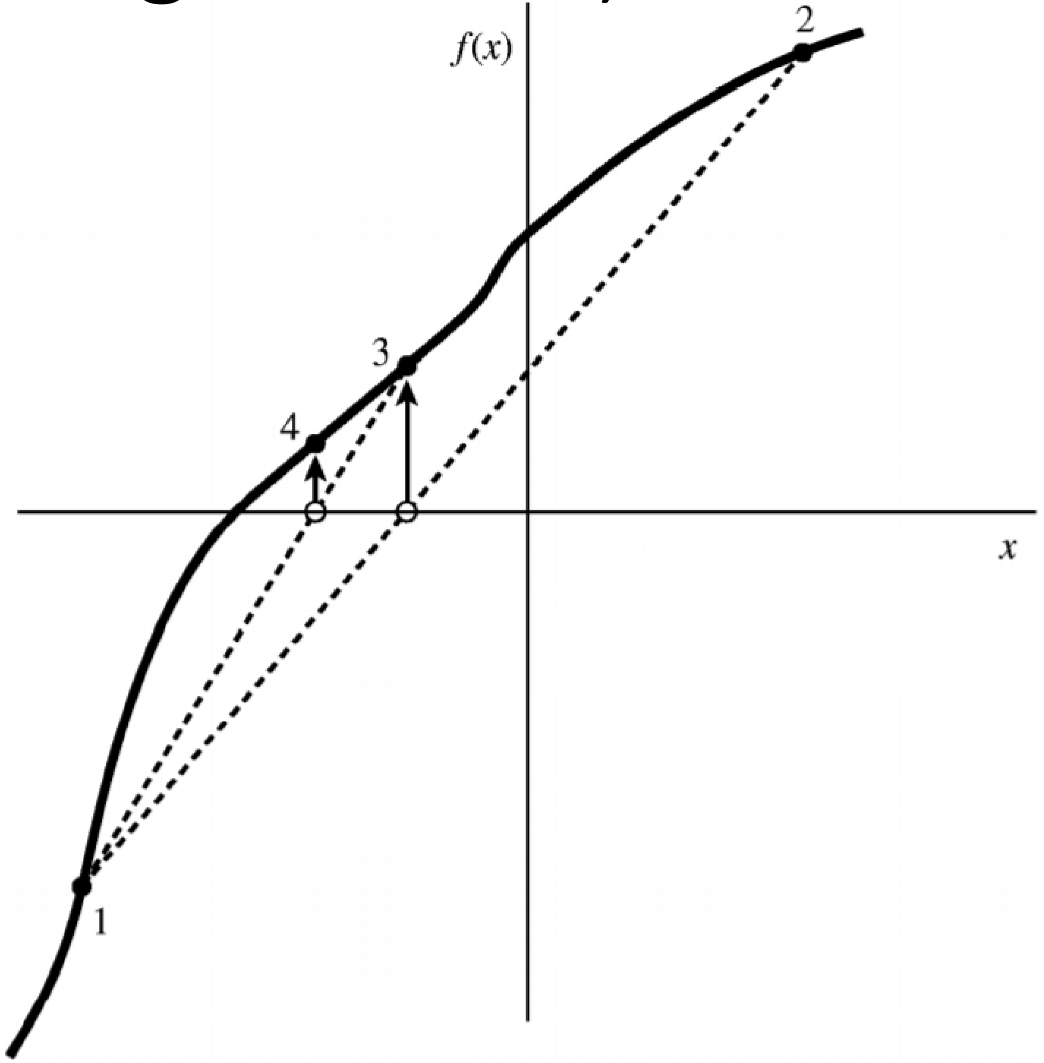


Figure 9.2.2. False position method. Interpolation lines (dashed) are drawn through the most recent points *that bracket the root*. In this example, point 1 thus remains "active" for many steps. False position converges less rapidly than the secant method, but it is more certain.

Slow convergence

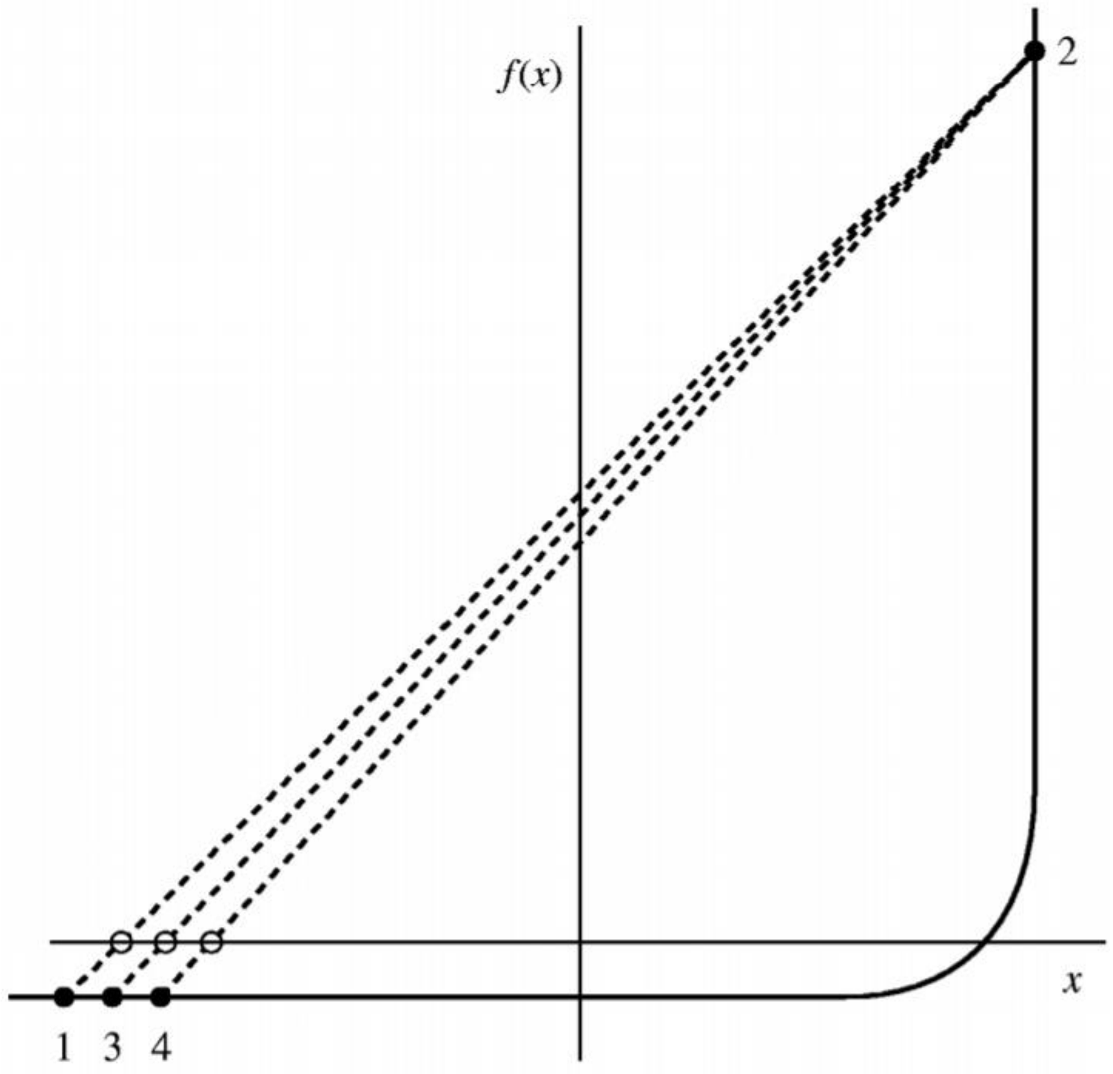


Figure 9.2.3. Example where both the secant and false position methods will take many iterations to arrive at the true root. This function would be difficult for many other root-finding methods.

Newton-Raphson method

- Pros:
  - Faster
  - Can be generalized to higher dimensions

$$\epsilon_{i+1} = -\epsilon_i^2 \frac{f''(x)}{2f'(x)}.$$

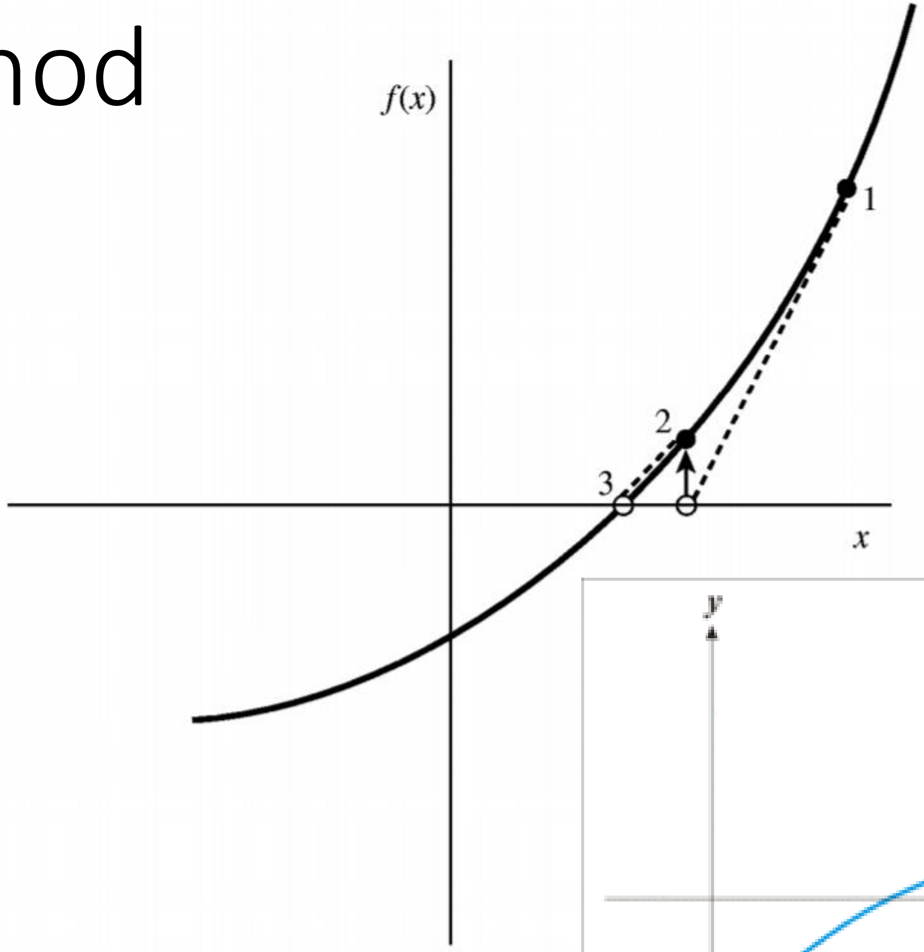
1D

$$\delta = -\frac{f(x)}{f'(x)}.$$

nD

$$\delta \mathbf{x} = -\mathbf{J}^{-1} \cdot \mathbf{F}$$

- Cons:
  - Not bracketed
  - Need derivative



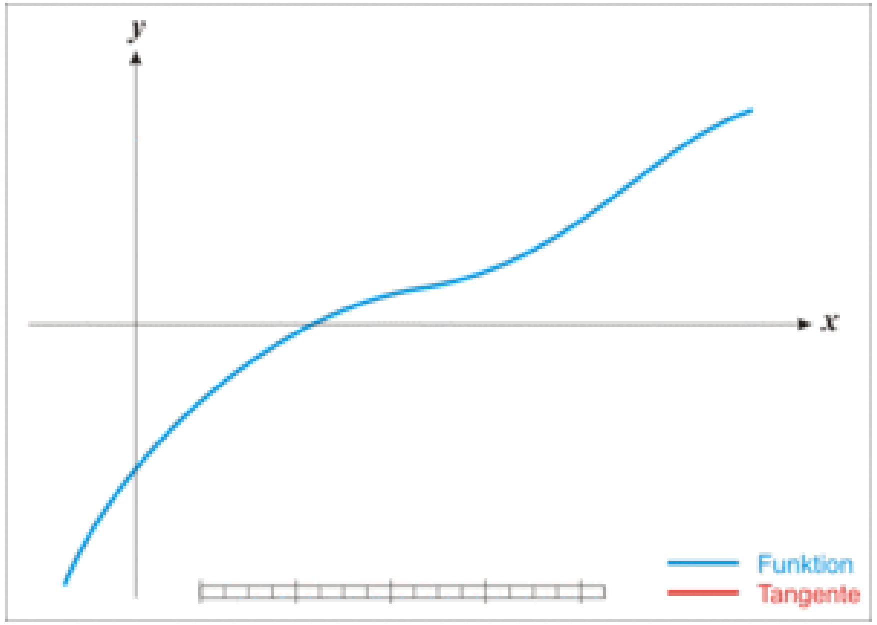
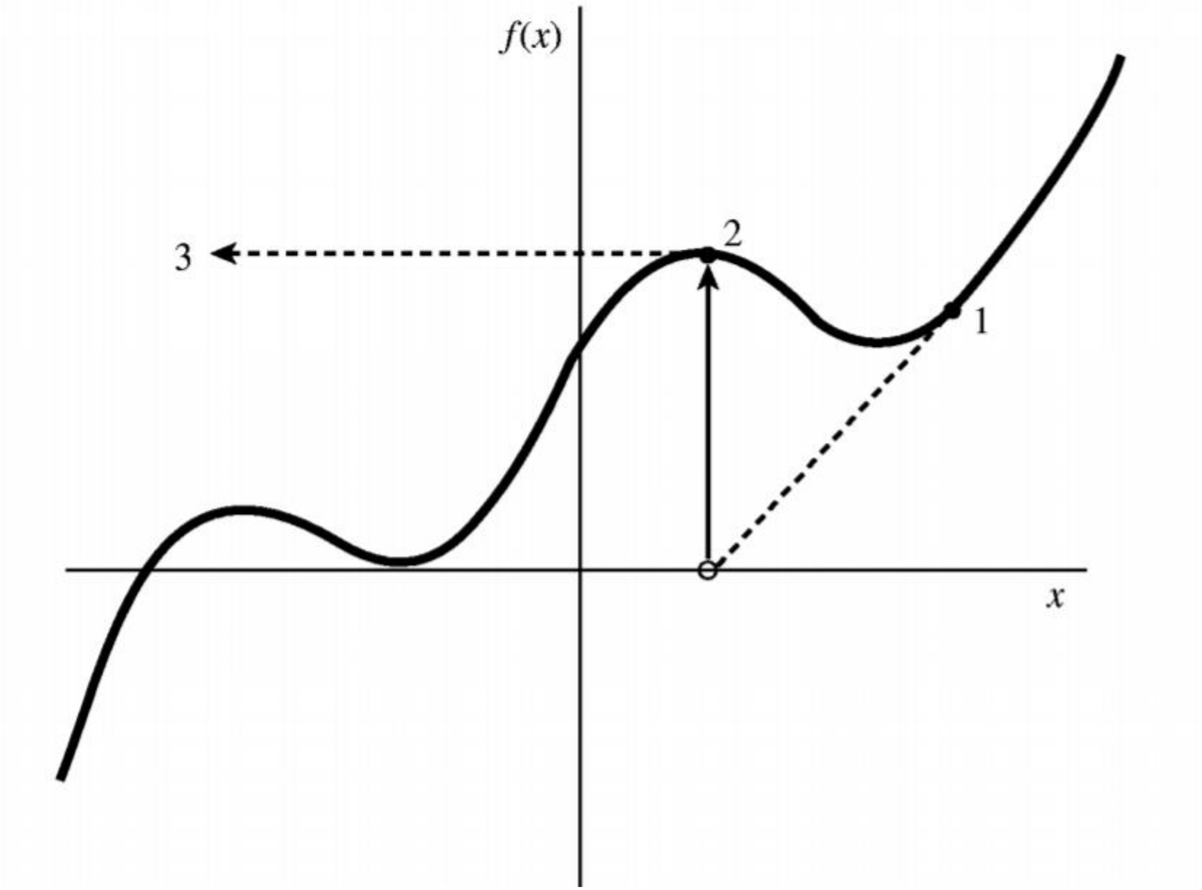
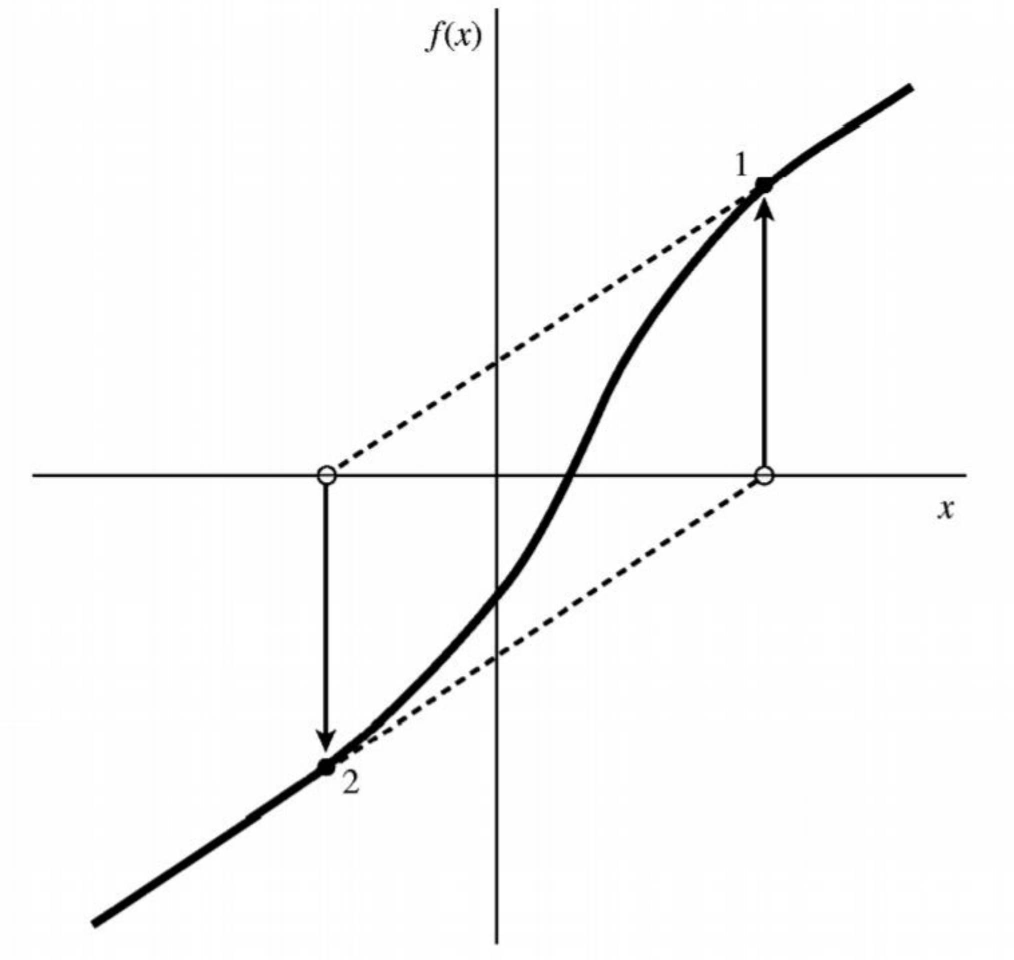


Figure 9.4.1. Newton's method extrapolates the local derivative to find the next estimate of the root. In this example it works well and converges quadratically.

Possible problematic cases

- Solution: combine with bracketing





Newton-Raphson higher dimensions (set of nonlin. Eqs.)

- 1D

$$f(x+\epsilon) = f(x) + \epsilon f'(x) + \epsilon^2 \frac{f''(x)}{2} + \cdots$$

$$\boxed{\delta = -\frac{f(x)}{f'(x)}.}$$

- nD

$$\mathbf{F}(\mathbf{x} + \delta\mathbf{x}) = \mathbf{F}(\mathbf{x}) + \mathbf{J} \cdot \delta\mathbf{x} + O(\delta\mathbf{x}^2).$$

$$\boxed{\delta\mathbf{x} = -\mathbf{J}^{-1} \cdot \mathbf{F}}$$

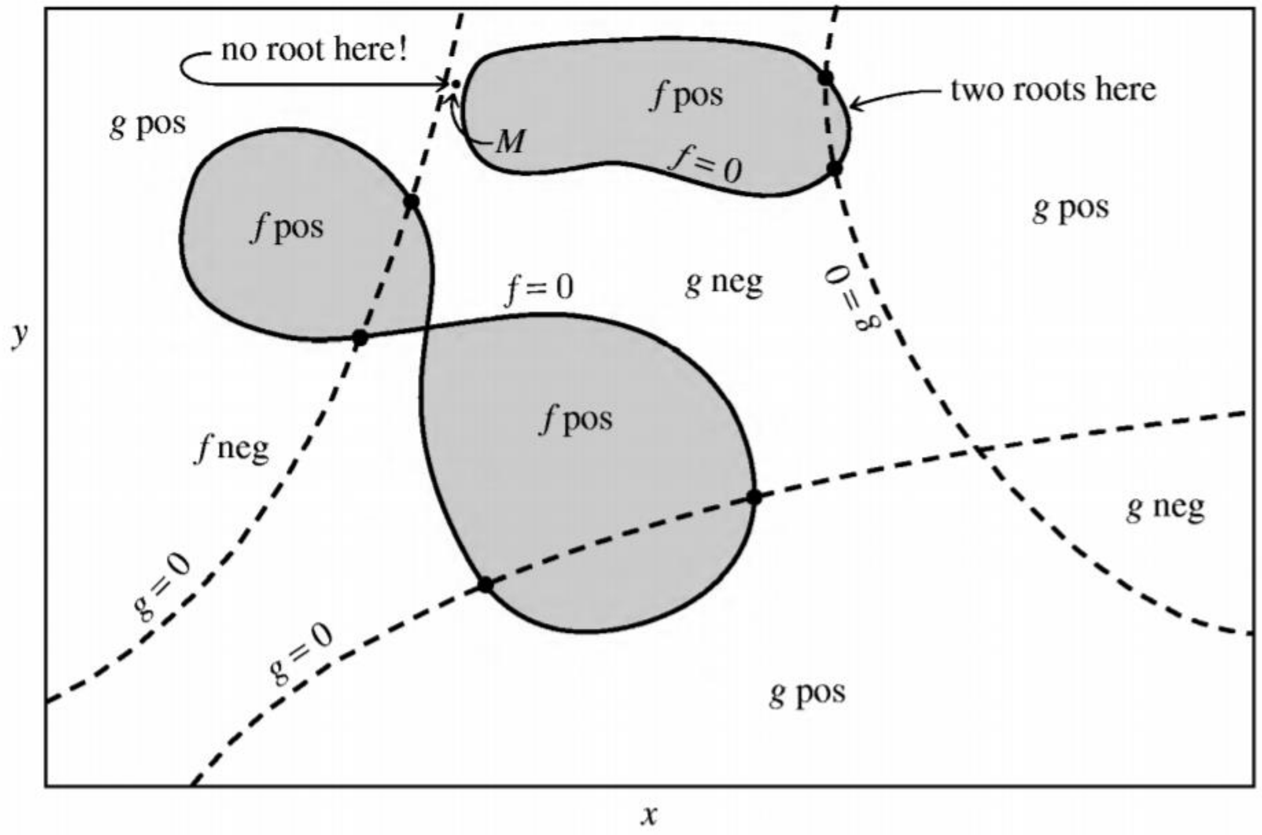


Figure 9.6.1. Solution of two nonlinear equations in two unknowns. Solid curves refer to $f(x, y)$, dashed curves to $g(x, y)$. Each equation divides the (x, y) plane into positive and negative regions, bounded by zero curves. The desired solutions are the intersections of these unrelated zero curves. The number of solutions is *a priori* unknown.