Numerical Methods

These notes are based on the Oxford Numerical Methods course taught by David Marshall (2023 for the NERC DTP) with additional context from LeVeque [1].

Contents

1 Root finding

Consider a function $f(x)$. If f is a quadratic polynomial, we may find the zeros of f using the quadratic formula, but for degrees 5 or larger, there exists no general formula for the zeros (Abel–Ruffini theorem). In general, finding an x^* such that $f(x^*) = 0$ cannot be computed exactly. Instead one must employ numerical root finding algorithms. Common methods include the bisection method and Newton's method.

1.1 Bisection method

Example 1.1

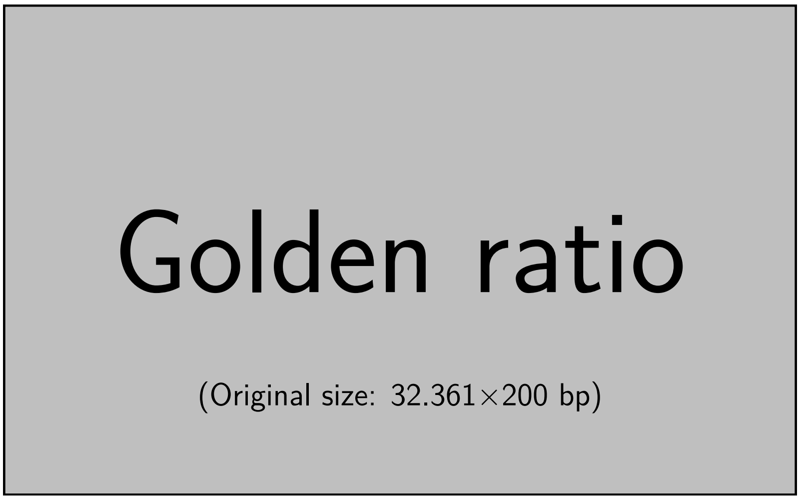

Figure 1: Bisection method

1.2 Newton's method

A quicker alternative to bisection is Newton's method (also known as Newton-Raphson). Given an initial guess x_0 and a sufficiently nice derivative f', we may estimate the zero x^* of f.

Consider the Taylor expansion of f around x_n (see Appendix A.1 for the big O notation and Appendix A.2 for Taylor):

$$f(x) = f(x_n) + f'(x_n)(x - x_n) + O((x - x_n)^2).$$

If we suppose that x_n is close to the root x^*, the zero of the linear approximation x_{n+1} is a good approximation for x^*

$$f(x_{n+1}) \approx 0 = f(x_n) + (x_{n+1} - x_n)f'(x_n).$$

Rearranging, we arrive at the iterative formula for Newton's method

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}. \tag{1}$$

This process is illustrated in Figure 2.

The error at iteration n is $\varepsilon_n = x_n - x^*$. By considering the quadratic term in the Taylor expansion around x_n, we get

$$\begin{aligned}
f(x^*) &= f(x_n) + f'(x_n)(x^* - x_n) + \frac{f''(x_n)}{2}(x^* - x_n)^2 + O((x^* - x_n)^3) \\
\implies \quad 0 &= f(x_n) + f'(x_n)(x^* - x_n) + \frac{f''(x_n)}{2}\varepsilon_n^2 + O(\varepsilon_n^3) \\
\implies \quad -\frac{f(x_n)}{f'(x_n)} &= (x^* - x_n) + \frac{f''(x_n)}{2}\varepsilon_n^2 + O(\varepsilon_n^3) \\
\implies \quad x_{n+1} - x_n &= (x^* - x_n) + \frac{f''(x_n)}{2}\varepsilon_n^2 + O(\varepsilon_n^3) \\
\implies \quad \varepsilon_{n+1} &= \frac{f''(x_n)}{2}\varepsilon_n^2 + O(\varepsilon_n^3)
\end{aligned}$$

Thus, as $n \to \infty$, $x_n \to x^*$ for a root x^* of f. In particular, we have quadratic convergence.

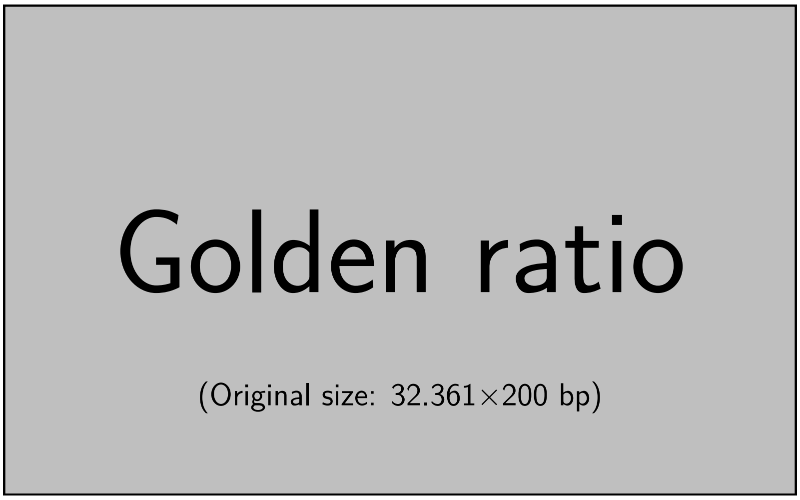

Figure 2: Newton's method

Example 1.2
The positive zero of the polynomial $f(x) = x^2 - 2$ can be approximated using Taylor's method with the starting guess $x_0 = 2$. Differentiating, $f'(x) = 2x$. Then we get

$$\begin{aligned}
x_1 &= x_0 - \frac{f(x_0)}{f'(x_0)} = 2 - \frac{2^2 - 2}{4} = 1.5 \\
x_2 &= 1.5 - \frac{1.5^2 - 2}{3} = 1.41666667 \\
x_3 &= 1.41421569 \\
x_4 &= 1.41421356 = \sqrt{2}.
\end{aligned}$$

Warning: if $f'(x_n) = 0$, Newton's method will not work (division by zero!) – pick a new x_0. If the derivative is not well behaved (either not defined or close to zero at many points), then Newton's method may not be appropriate.

1.3 Higher dimensions

Consider the system of m equations in n variables $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ given by

$$\begin{cases}
f_1(x_1, x_2, \ldots, x_n) = 0, \\
f_2(x_1, x_2, \ldots, x_n) = 0, \\
\qquad\qquad \vdots \\
f_m(x_1, x_2, \ldots, x_n) = 0.
\end{cases}$$

2 Finite difference

3 Von Neumann analysis

4 Numerical linear algebra

A Background theory

A.1 Big O notation

A.2 Taylor expansions

Theorem A.1 (Taylor)

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \cdots$$

References

[1] R. J. LeVeque. *Finite difference methods for ordinary and partial differential equations: steady-state and time-dependent problems.* Society for Industrial and Applied Mathematics, Philadelphia, PA, 2007.