Calculus is certainly one of the pillars of modern science and the cornerstone to most applications of mathematics in other disciplines. In order to apply its basic ideas to real world problems, additional study of subjects such as differential equations and numerical analysis is eventually needed. However, the authors feel that short introductions to these topics, rather than scare the students, may show them the benefits of mastering the mathematical computational tools presented in this book.

9.1 Introduction

A numerical method is a model for solving a problem for which a solution consists of calculating one or several numbers. For example, a numerical method to find an approximate to the derivative $f'(x)$ is to calculate $f(x+h), f(x-h)$ for a "small" $h$ and take

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

The quality of this approximation depends on the size of $h$ and we can show that

$$\lim_{h \to 0} \frac{f(x+h) - f(x-h)}{2h} = f'(x)$$

Usually, we want to approximate a solution to a problem within some desired degree of precision or tolerance. The first step is finding a numerical method that can perform that task. Then, we design an algorithm, based on this method, which is a finite sequence of steps that need to be executed in order to obtain the approximate solution. We emphasize the word finite since whether we use a pencil, a calculator or a computer, we must confine ourselves to a finite number of arithmetic operations. The number of operations may increase if a higher accuracy is requested, but it will always stay finite.

Example 9.1.1. In order to solve the linear equation $ax + b = c$ with arbitrary coefficients $a, b, c$ we can use the following algorithm:
Step 1. Calculate \( d = c - b \).

Step 2. If \( a = 0 \) write ‘there is no solution’ and stop; If \( a \neq 0 \) calculate \( x = \frac{d}{a} \) and stop.

Example 9.1.2. Consider the problem of finding the square root of a given \( a > 1 \). An efficient numerical method for calculating an approximate to \( \sqrt{a} \), is to create the sequence

\[
x_0 = a; \quad x_n = \frac{1}{2} \left( x_{n-1} + \frac{a}{x_{n-1}} \right), \quad n \geq 1
\]

The process of calculating each \( x_n \) is called iteration and we often use this term for the number \( x_n \) as well. Since \( \{x_n\} \) is a monotone decreasing sequence (why?) and \( \lim_{n \to \infty} x_n = \sqrt{a} \) (for details see Section 9.3 below), this method enables us to approximate \( \sqrt{a} \) to any given degree of precision. The algorithm designed for this purpose will be formulated next, after we set an agreeable definition for convergence for our problem.

Given an approximate \( s \) to \( \sqrt{a} \), we measure its accuracy by the distance \( |s - \sqrt{a}| \). Let \( \epsilon > 0 \) denote a prefixed desired tolerance. Unfortunately, we do not know \( \sqrt{a} \) and are unable to compute \( |s - \sqrt{a}| \). However, since

\[
|s^2 - a| = |s - \sqrt{a}| |s + \sqrt{a}| \geq 2\sqrt{a} |s - \sqrt{a}| \geq 2|s - \sqrt{a}|
\]

we may replace the convergence test defined here by the inequality \( |s - \sqrt{a}| < \epsilon \), by the stronger request \( |s^2 - a| < 2\epsilon \) which implies \( |s - \sqrt{a}| < \epsilon \) (why?). The algorithm can be represented as follows:

Step 1. Given an arbitrary positive number \( a > 1 \) and a desired tolerance \( \epsilon > 0 \), choose an initial approximate to \( \sqrt{a} \) (from above), say \( x_0 = a \) and set \( n = 0 \).

Step 2. Use Eq. (9.1.1) to get the iteration \( x_{n+1} \).

Step 3. If \( |x_{n+1}^2 - a| < 2\epsilon \) the computation is over and \( x_{n+1} \) is taken as the final approximate to \( \sqrt{a} \). The total number of iterations needed for convergence is \( n + 1 \); If \( |x_{n+1}^2 - a| \geq 2\epsilon \) set \( n \leftarrow n + 1 \) and go to Step 2.