Self Assignment: Applications of Scientific Computing

2024

Introduction

Numerical methods are mathematical tools used for approximating solutions to complex problems in scientific computing. These methods are critical in fields like physics, engineering, biology, and finance. In this lecture, we will cover some basic numerical methods, explain their applications, and provide simple examples.

1 Numerical Methods Overview

Numerical methods allow computers to handle mathematical problems that do not have exact solutions or are too complex for analytical solutions. Some common numerical methods include:

- **Root Finding Methods** - Methods like Bisection and Newton-Raphson that help find solutions to equations.
- **Numerical Integration** - Approximating the area under a curve, such as with Trapezoidal and Simpson's rule.
- **Solving Differential Equations** - Methods like Euler's Method and Runge-Kutta for approximating solutions to differential equations.
- **Linear Algebra** - Solving systems of linear equations using techniques like Gaussian Elimination or LU Decomposition.

Each method simplifies real-world problems to a form that can be computed on modern computers.

2 Root Finding: Newton's Method

Newton's Method is a simple and powerful way to find where a function equals zero. In other words, it helps us find the root of a function, which is the point where the function crosses the x-axis.

The method works by starting with a guess and refining it using the slope (or derivative) of the function. The formula for updating the guess is:

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

Where:

- x_n is the current guess.
- $f(x_n)$ is the value of the function at x_n.
- $f'(x_n)$ is the slope (or derivative) of the function at x_n.

Example: Let's find the square root of 2 using Newton's Method. The problem can be written as $f(x) = x^2 - 2$, and we want to find the value of x where $f(x) = 0$. The derivative of this function is $f'(x) = 2x$.

We start with an initial guess of $x_0 = 1$. Now we apply the formula:

$$x_1 = 1 - \frac{1^2 - 2}{2(1)} = 1 - \frac{-1}{2} = 1.5$$

So, our next guess is $x_1 = 1.5$.

We repeat the process to refine the guess further:

$$x_2 = 1.5 - \frac{1.5^2 - 2}{2(1.5)} = 1.5 - \frac{0.25}{3} \approx 1.41667$$

After two iterations, we have $x_2 \approx 1.41667$, which is very close to $\sqrt{2}$.

This process can be repeated to get even more accurate results, but already, after just two steps, we've found a value close to the square root of 2.

3 Numerical Integration: Trapezoidal Rule

Numerical integration is used to estimate the value of definite integrals when they cannot be solved exactly. The Trapezoidal Rule is a simple technique that approximates the area under a curve by dividing the interval into small trapezoids, instead of rectangles. This provides a better approximation compared to simple methods like Riemann sums.

3.1 Trapezoidal Rule Formula

The Trapezoidal Rule works by connecting two points on the curve with a straight line, forming a trapezoid, and calculating the area of that trapezoid. The formula for the Trapezoidal Rule when approximating the integral of a function $f(x)$ over the interval $[a, b]$ is:

$$\int_a^b f(x)dx \approx \frac{b-a}{2}\left[f(a) + f(b)\right]$$

Where:

- a and b are the endpoints of the interval.
- $f(a)$ is the function evaluated at the left endpoint.
- $f(b)$ is the function evaluated at the right endpoint.

3.2 Why Trapezoidal Rule Works

Instead of calculating the exact area under the curve, which may be complicated or impossible, we approximate it using trapezoids. Each trapezoid provides an approximation to the area, and the sum of these small areas gives us the total estimated area under the curve.

Example: Approximating $\int_0^1 x^2 dx$

Let's apply the Trapezoidal Rule to approximate the integral:

$$\int_0^1 x^2 dx$$

We want to estimate the area under the curve $f(x) = x^2$ between $x = 0$ and $x = 1$.

1. First, we calculate the values of the function at the endpoints:

$$f(0) = 0^2 = 0 \quad \text{and} \quad f(1) = 1^2 = 1$$

2. Using the Trapezoidal Rule formula, we approximate the integral:

$$\int_0^1 x^2 dx \approx \frac{1-0}{2}\left[f(0) + f(1)\right] = \frac{1}{2}[0+1] = \frac{1}{2}$$

The exact value of the integral is:

$$\int_0^1 x^2 dx = \frac{1}{3}$$

The Trapezoidal Rule gives us a close approximation of $\frac{1}{2}$, which demonstrates how it works as a rough but useful estimate.

3.3 Improving the Trapezoidal Rule

To get a more accurate result, you can divide the interval into smaller segments (sub-intervals), apply the Trapezoidal Rule to each sub-interval, and sum the areas of all the trapezoids. This will give a better approximation of the integral.

$$\int_a^b f(x)dx \approx \frac{h}{2}\left[f(x_0) + 2f(x_1) + 2f(x_2) + \cdots + 2f(x_{n-1}) + f(x_n)\right]$$

where h is the width of each sub-interval.

4 Solving Differential Equations: Euler's Method

Euler's Method is a simple and intuitive way to approximate the solutions to first-order ordinary differential equations (ODEs). In many real-world situations, we can't solve ODEs exactly, so we use methods like Euler's Method to estimate the solution at different points.

4.1 The Basic Idea

Given a differential equation of the form:

$$y'(x) = f(x, y), \quad y(x_0) = y_0$$

Euler's Method works by stepping forward in small increments, using the slope of the function to estimate the next point. The formula for updating the solution is:

$$y_{n+1} = y_n + h \cdot f(x_n, y_n)$$

Where:

- y_n is the current value of the solution.
- x_n is the current value of x.
- h is the step size, or the distance between consecutive x-values.
- $f(x_n, y_n)$ gives the slope of the function at the current point.

The smaller the step size h, the more accurate the approximation will be, but it will also require more steps to reach the desired x-value.

Example: Solving $y'(x) = -2x$ with Euler's Method

Let's use Euler's Method to approximate the solution to the differential equation:

$$y'(x) = -2x, \quad y(0) = 1$$

We want to estimate $y(1)$, and we'll use a step size of $h = 0.1$.

1. **Initial condition**: $y(0) = 1$, so our starting point is $(x_0, y_0) = (0, 1)$. 2. **First step**: Using the formula for Euler's Method, we calculate:

$$y_1 = y_0 + h \cdot f(x_0, y_0) = 1 + 0.1 \cdot (-2 \cdot 0) = 1$$

So after the first step, we have $(x_1, y_1) = (0.1, 1)$. 3. **Second step**: Now, we calculate the next value:

$$y_2 = y_1 + h \cdot f(x_1, y_1) = 1 + 0.1 \cdot (-2 \cdot 0.1) = 1 + 0.1 \cdot (-0.2) = 0.98$$

So after the second step, we have $(x_2, y_2) = (0.2, 0.98)$.

Repeating this process step by step will give us approximate values of $y(x)$ at different points. For example, after 10 steps, we'll have an approximation for $y(1)$.

4.2 How Euler's Method Works

Euler's Method essentially moves along the curve by taking small steps. At each step, it uses the slope of the curve (given by the differential equation) to estimate the value of the solution at the next point.

4.3 Accuracy of Euler's Method

The accuracy of Euler's Method depends on the step size h. Smaller step sizes lead to better approximations, but require more steps. For more complex problems, more advanced methods like the Runge-Kutta method are used to get better accuracy with fewer steps.

4.4 Visualization

Imagine a curve, and at each point on the curve, there is a tangent line. Euler's Method follows this tangent line for a small step, then recalculates the slope and follows the next tangent. This way, it approximates the curve step by step, giving us a sequence of points that approximate the solution.