Introduction to Computational Physics

UPES Dehradun

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Dr. Nitesh Kumar

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Contents

Chapter 1

Introduction to FORTRAN 90 on Linux

1.1 Getting Started with Linux

Before diving into FORTRAN 90, it's essential to understand some basic Linux commands and environment setup to efficiently work with programming on Linux. Linux is a powerful and flexible operating system that is widely used for programming and scientific computing.

1.1.1 Basic Linux Commands

Here are some basic Linux commands you'll use frequently while working with FORTRAN and other programming languages:

- `pwd`: Print the current working directory.

```
$ pwd
/home/user

```

- `ls`: List files and directories.

```
$ ls
Documents  Downloads  hello.f90  Pictures

```

- `cd`: Change directory.

```
$ cd Documents

```

- `mkdir`: Create a new directory.

```
$ mkdir fortran_projects

```

- `rm`: Remove files or directories.

```
$ rm hello.f90

```

- `nano` or `vim`: Command-line text editors. We'll use `nano` for simplicity.

```
$ vim hello.f90

```

- `gfortran`: The GNU Fortran compiler, used for compiling FORTRAN code.

1.1.2 File System Hierarchy

Linux organizes files and directories into a hierarchical structure, starting with the root directory (`/`). Some common directories you'll work with include:

- `/home`: Contains user home directories.
- `/usr`: Contains installed software and libraries.
- `/etc`: Configuration files.

Understanding this structure will help you navigate and manage files while working on your projects.

1.2 Historical Development of FORTRAN

FORTRAN (FORmula TRANslation) is one of the oldest high-level programming languages. Originally developed in the 1950s by IBM, it has evolved significantly over the decades, with FORTRAN 90 being a major revision.

1.2.1 Evolution of FORTRAN

- **FORTRAN I (1957)**: The first compiled high-level language, primarily designed for scientific and engineering computations.
- **FORTRAN IV and 66 (1960s)**: Introduced subroutines, functions, and better control structures.
- **FORTRAN 77**: Improved string handling and more complex control structures.
- **FORTRAN 90 (1991)**: Introduced modern programming concepts like recursion, modules, dynamic memory allocation, and array programming.

FORTRAN 90 represents a significant step forward from FORTRAN 77, incorporating many new features designed to improve the flexibility and readability of code.

1.3 Setting Up the FORTRAN Environment on Linux

Before writing any code, you need to install the GNU Fortran compiler. Most Linux distributions provide the `gfortran` package.

1.3.1 Installing GNU Fortran Compiler (gfortran)

To install `gfortran` on a Debian-based system (like Ubuntu), run:

```
$ sudo apt-get update
$ sudo apt-get install gfortran
```

For Red Hat-based systems, use:

```
$ sudo yum install gfortran
```

After installation, you can check if the compiler is installed correctly:

```
$ gfortran --version
```

1.4 Introduction to Fortran

Fortran (short for Formula Translation) is a general-purpose, imperative programming language that is particularly suited for scientific and engineering applications. It was developed in the 1950s and has since evolved into several versions, with Fortran 90 and Fortran 95 being the most widely used.

1.4.1 Basic Syntax

Fortran programs are composed of statements, which are written in a fixed-format style. Each statement begins in column 1 and can extend up to column 72. Statements are typically written in uppercase, although lowercase is also allowed.

1.4.2 Variables and Data Types

Fortran supports several data types, including integers, real numbers, complex numbers, and character strings. Variables are declared using the `INTEGER`, `REAL`, `COMPLEX`, or `CHARACTER` keywords, followed by the variable name.

1.4.3 Control Structures

Fortran provides various control structures for program flow, including `IF-THEN-ELSE` statements, `DO` loops, and `SELECT CASE` statements. These structures allow for conditional execution and repetitive tasks.

1.4.4 Arrays

Arrays are an essential part of Fortran programming. They allow you to store and manipulate multiple values of the same data type. Fortran supports both one-dimensional and multi-dimensional arrays.

1.4.5 Subroutines and Functions

Subroutines and functions are used to modularize code and improve code reusability. Subroutines are blocks of code that perform a specific task, while functions return a value.

1.4.6 File Handling

Fortran provides built-in functions and subroutines for reading from and writing to files. This allows you to interact with external data files and perform input/output operations.

1.5 Advanced Topics

Fortran also offers advanced features such as modules, derived types, and object-oriented programming. These features enhance code organization and allow for more complex programming structures.

1.6 Example Programs

1.6.1 Basic syntax

```
PROGRAM hello
  PRINT *, 'Hello, World!'
END PROGRAM hello
```

To compile the program, use the following commands:

```
$ gfortran hello.f90 -o hello
```

To run the compiled program, use:

```
$ ./hello
```

Output:

```
Hello, World!
```

1.6.2 Variables and data types

```
PROGRAM variables
  INTEGER :: i
  REAL :: x
  COMPLEX :: z
  CHARACTER(LEN=10) :: name
  LOGICAL ::

  i = 10
  x = 3.14
  z = (1.0, 2.0)
  name = 'Fortran'

  PRINT *, 'Integer:', i
  PRINT *, 'Real:', x
  PRINT *, 'Complex:', z
  PRINT *, 'Character:', name
END PROGRAM variables
```


To compile the program, use the following commands:

```
$ gfortran variables.f90 -o variables
```

To run the compiled program, use:

```
$ ./variables
```

Output:

```
Integer:           10
Real:     3.14000000
Complex:    (1.00000000,2.00000000)
Character: Fortran
```

1.6.3 Control structures

```
PROGRAM control
  INTEGER :: i
  i = 5

  IF (i > 0) THEN
    PRINT *, 'Positive'
  ELSE
    PRINT *, 'Negative'
  END IF

  DO i = 1, 5
    PRINT *, i
  END DO

  SELECT CASE (i)
    CASE (1)
      PRINT *, 'One'
    CASE (2)
      PRINT *, 'Two'
    CASE DEFAULT
      PRINT *, 'Other'
  END SELECT
END PROGRAM control
```

To compile the program, use the following commands:

```
$ gfortran control.f90 -o control
```

To run the compiled program, use:

```
$ ./control
```

Output:

```
Positive
           1
           2
```



```
            3
            4
            5
Other
```

1.6.4 Arrays

```
PROGRAM arrays
  INTEGER, DIMENSION(3) :: a
  REAL, DIMENSION(2, 2) :: b

  a = [1, 2, 3]
  b = RESHAPE([1.0, 2.0, 3.0, 4.0], [2, 2])

  PRINT *, 'Array a:', a
  PRINT *, 'Array b:'
  DO i = 1, 2
    PRINT *, b(i, :)
  END DO
END PROGRAM arrays
```

To compile the program, use the following commands:

```
$ gfortran arrays.f90 -o arrays
```

To run the compiled program, use:

```
$ ./arrays
```

Output:

```
Array a:           1           2           3
Array b:
   1.00000000        2.00000000
   3.00000000        4.00000000
```

1.6.5 Functions

The syntax of the function is given below.

```
    type FUNCTION func-name(arg1, arg2, ....)
        IMPLICIT NONE
        [specification part]
        [execution part]
        [subprogram part]
    END FUNCTION func-name
```

where 'type' is the data types like 'INTEGER', 'REAL', ... etc.

A sample code to add two numbers using Fortran function is given below:

```
program adding
        IMPLICIT NONE
        INTEGER :: a, b, addition, add
```



```
        a = 4
        b = 6
        addition = add(a, b)
        print*, a, b, addition
END PROGRAM adding

INTEGER FUNCTION add(x, y)
        IMPLICIT NONE
        INTEGER, INTENT(IN) :: x, y
        add = (x+y)
END FUNCTION add
```

Another way of writing functions in Fortran:

```
program TwoFunctions
        IMPLICIT NONE
        REAL :: a, b, A_mean, G_mean
        READ(*,*) a, b
        A_mean = ArithMean(a, b)
        G_mean = GeoMean(a, b)
        WRITE(*,*) a, b, A_mean, G_Mean
CONTAINS
        REAL FUNCTION ArithMean(a, b)
                IMPLICIT NONE
                REAL, INTENT(IN) ::a, b
                ArithMean = (a+b)/2.0
        END FUNCTION ArithMean

        REAL FUNCTION GeoMean(a, b)
                IMPLICIT NONE
                REAL, INTENT(IN) ::a, b
                GeoMean = SQRT(a*b)
        END FUNCTION GeoMean
END PROGRAM TwoFunctions
```

1.6.6 Subroutines

```
PROGRAM main
  IMPLICIT NONE
  INTEGER :: x, y, z
  x = 5
  y = 2
  CALL ADD(x, y, z)
  print*, 'ADDITION IS', z
END PROGRAM main

SUBROUTINE ADD(a, b, c)
  IMPLICIT NONE
  INTEGER, INTENT(IN) :: a, b
  INTEGER, INTENT(OUT) :: c
  c = a + b
```

```
END SUBROUTINE ADD
```

To compile the program, use the following commands:

```
$ gfortran main.f90 -o main
```

To run the compiled program, use:

```
$ ./main
```

Output:

```
Sum:           15
```

1.6.7 File handling

This code demonstrates how to write data to a file in Fortran. It opens a file, writes multiple lines to it, and then closes the file.

```
PROGRAM write_to_file
  INTEGER :: unit_number
  INTEGER :: i
  CHARACTER(len=20) :: filename

  ! Set the file name and the unit number
  filename = 'output.txt'
  unit_number = 10

  ! Open the file for writing
  OPEN(unit=unit_number, file=filename, status='unknown')

  ! Write some data into the file
  DO i = 1, 5
     WRITE(unit_number, *) 'Line number:', i
  END DO

  ! Close the file
  CLOSE(unit_number)

  PRINT *, 'Data has been written to ', filename
END PROGRAM write_to_file
```

Explanation

- `PROGRAM write_to_file`: The program starts with a main program block named `write_to_file`.
- `INTEGER :: unit_number, i`: The variables `unit_number` and `i` are declared as integers. `unit_number` represents the file identifier, and `i` is used in the loop.
- `CHARACTER(len=20) :: filename`: This declares a character variable `filename` with a length of 20 characters to store the name of the file.

- `OPEN(unit=unit_number, file=filename, status='unknown')`: Opens the file `output.txt` with the file unit specified by `unit_number`. The `status='unknown'` allows Fortran to create the file if it doesn't exist or overwrite it if it already exists.
- `DO i = 1, 5`: This loop runs from 1 to 5, writing a line to the file in each iteration.
- `WRITE(unit_number, *) 'Line number:', i`: This statement writes the text `'Line number:'` followed by the value of `i` to the file.
- `CLOSE(unit_number)`: Closes the file associated with `unit_number`.

To compile the program, use the following commands:

```
$ gfortran file_handling.f90 -o file_handling
```

To run the compiled program, use:

```
$ ./file_handling
```

These example programs demonstrate the basic syntax, variables, control structures, arrays, subroutines, functions, and file handling in Fortran programming. By understanding these concepts, you can start writing your own Fortran programs for scientific and engineering applications.

1.7 Linking external libraries

Linking to external libraries in Fortran is a common task when you want to leverage precompiled libraries such as LAPACK, BLAS, or others for numerical and scientific computations. This document will explain the steps to link Fortran programs with external libraries using the GNU Fortran compiler (`gfortran`), and provide an example of linking to the LAPACK library.

1.7.1 Steps to Link to External Libraries

To link an external library to your Fortran program, follow these steps:

1. **Install the necessary libraries:** Ensure that the external library is installed on your system. For example, you can install LAPACK and BLAS on Linux using the following command:

```
    sudo apt-get install liblapack-dev libblas-dev

```

2. **Compile the Fortran code:** Use the `gfortran` compiler to compile your Fortran code and link it to the library using the `-l` option.
3. **Link during compilation:** Use the `-L` option to specify the path to the external library and the `-l` option to link against the library.

1.7.2 Example: Solving a Linear System using LAPACK

Below is an example Fortran program that solves a system of linear equations $Ax = b$ using the LAPACK routine `dgesv`, which performs LU decomposition.

1.7.3 Fortran Code

```
PROGRAM solve_linear_system
  USE, INTRINSIC :: iso_c_binding
  IMPLICIT NONE

  INTEGER, PARAMETER :: n = 3
  INTEGER :: info
  REAL(KIND=c_double), DIMENSION(n,n) :: A
  REAL(KIND=c_double), DIMENSION(n) :: B
  INTEGER, DIMENSION(n) :: ipiv

  ! Matrix A (3x3)
  A = RESHAPE([3.0d0, 1.0d0, 2.0d0, &
               6.0d0, 3.0d0, 4.0d0, &
               9.0d0, 5.0d0, 8.0d0], [n,n])

  ! Right-hand side vector B (3x1)
  B = [1.0d0, 0.0d0, 2.0d0]

  ! Call LAPACK subroutine to solve the system of equations A*x =
    B
  CALL dgesv(n, 1, A, n, ipiv, B, n, info)

  ! Check for errors
  IF (info /= 0) THEN
    PRINT *, 'Error: LAPACK dgesv failed with info =', info
  ELSE
    PRINT *, 'Solution vector X:'
    PRINT *, B
  END IF

END PROGRAM solve_linear_system
```

In this program:

- The matrix A is a 3x3 matrix, and B is a 3x1 vector. The goal is to solve $Ax = B$ for the unknown vector x.
- `dgesv` is the LAPACK routine that performs the LU decomposition and solves the system of equations.

Explanation

- `PROGRAM solve_linear_system`: This statement starts the main program block named `solve_linear_system`.
- `USE, INTRINSIC :: iso_c_binding`: This module provides definitions for interoperability with C, particularly for specifying precision with `c_double`.
- `IMPLICIT NONE`: This directive requires explicit declaration of all variables, helping to avoid errors due to undeclared variables.

- `INTEGER, PARAMETER :: n = 3`: This declares an integer parameter `n` with a value of 3, representing the size of the matrix and vector.
- `INTEGER :: info`: This integer variable will store the error information returned by the LAPACK subroutine.
- `REAL(KIND=c_double), DIMENSION(n,n) :: A`: Declares a 3x3 matrix `A` of type `REAL(KIND=c_double)` for high-precision floating-point numbers.
- `REAL(KIND=c_double), DIMENSION(n) :: B`: Declares a 3x1 vector `B` of the same floating-point type.
- `INTEGER, DIMENSION(n) :: ipiv`: Declares an integer array `ipiv` used by the LAPACK subroutine to store pivot indices.
- `A = RESHAPE([...] [,n,n])`: Initializes the matrix `A` with specific values and reshapes it to a 3x3 matrix.
- `B = [1.0d0, 0.0d0, 2.0d0]`: Initializes the vector `B` with given values.
- `CALL dgesv(n, 1, A, n, ipiv, B, n, info)`: Calls the LAPACK subroutine `dgesv` to solve the system of linear equations `A*x = B`. Here, `n` is the size of the matrix, `1` is the number of right-hand sides, `A` is the coefficient matrix, `ipiv` is the pivot index array, `B` is the right-hand side vector, and `info` will hold the exit status.
- `IF (info /= 0)`: Checks if the LAPACK subroutine encountered an error. If `info` is not zero, an error message is printed.
- `PRINT *, 'Solution vector X:'`: If there is no error, the solution vector `B` is printed, which contains the solution to the system.
- `END PROGRAM solve_linear_system`: Ends the program.

1.7.4 Compilation and Linking

To compile and link the program with the LAPACK and BLAS libraries, use the following commands:

```
gfortran solve_linear_system.f90 -o solve_linear_system -llapack
   -lblas
```

Here:

- `-llapack` links the LAPACK library.
- `-lblas` links the BLAS library, which is a prerequisite for LAPACK.

If the libraries are not in the default location, you can specify the path using the `-L` option:

```
gfortran solve_linear_system.f90 -o solve_linear_system -L/usr/
   local/lib -llapack -lblas
```


1.7.5 Running the Program

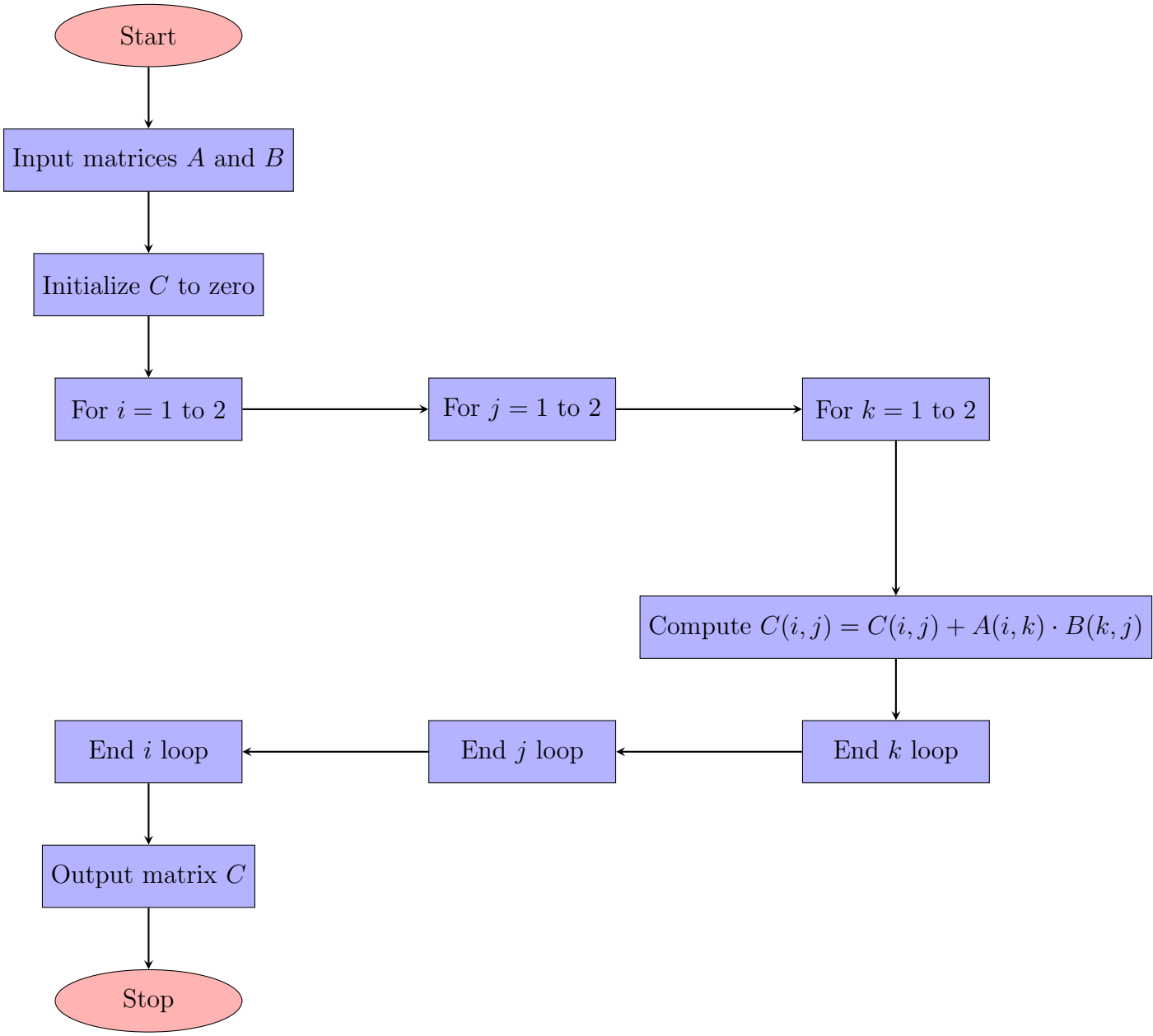
Once the program is compiled, you can run it using:

```
./solve_linear_system
```

The output will display the solution vector x for the system $Ax = b$.

1.8 Matrix Multiplication of size 2x2

1.8.1 Flowchart



1.8.2 Code

```
program matrix_multiplication
    implicit none
```



```
    real :: A(2, 2), B(2, 2), C(2, 2)

    ! Input matrices
    A = reshape([1.0, 2.0, 3.0, 4.0], shape(A))  ! Matrix A
    B = reshape([5.0, 6.0, 7.0, 8.0], shape(B))  ! Matrix B

    ! Call the function to multiply A and B, storing the result
   in C
    C = matrix_multiply(A, B)

    ! Output the result
    print *, "Matrix A:"
    call print_matrix(A)
    print *, "Matrix B:"
    call print_matrix(B)
    print *, "Resultant Matrix C (A * B):"
    call print_matrix(C)

contains

    ! Function to multiply two 2x2 matrices
    function matrix_multiply(A, B) result(C)
        implicit none
        real, intent(in) :: A(2, 2), B(2, 2)
        real :: C(2, 2)
        integer :: i, j, k

        ! Initialize the result matrix C to zero
        C = 0.0

        ! Perform matrix multiplication
        do i = 1, 2
            do j = 1, 2
                do k = 1, 2
                    C(i, j) = C(i, j) + A(i, k) * B(k, j)
                end do
            end do
        end do
    end function matrix_multiply

    ! Subroutine to print a 2x2 matrix
    subroutine print_matrix(M)
        implicit none
        real, intent(in) :: M(2, 2)
        integer :: i

        do i = 1, 2
            write(*, '(F6.2, F6.2)') M(i, 1), M(i, 2)
        end do
    end subroutine print_matrix

```

```
53 end program matrix_multiplication
```

1.9 Conclusion

This chapter introduced you to the basics of working with Linux and FORTRAN 90. You learned how to navigate the Linux file system, write a simple "Hello, World!" program, and compile and execute FORTRAN code using the `gfortran` compiler. In subsequent chapters, we'll dive deeper into advanced FORTRAN features such as arrays, file handling, and scientific computing techniques.

Exercise

Category 1: Easy (Conceptual and Memory-Based)

1. What makes Linux a preferred operating system for scientific computing?
2. Why is FORTRAN still relevant for numerical and scientific applications in the modern era?
3. What is the primary purpose of the `gfortran` compiler in FORTRAN programming?
4. Explain the difference between fixed-format and free-format styles in FORTRAN.
5. Why is the `IMPLICIT NONE` directive critical for error-free programming in FORTRAN?
6. What does the `RESHAPE` function do in FORTRAN? Provide an example scenario.
7. Define the purpose of modules in FORTRAN. How do they improve code organization?
8. Why are control structures such as `DO` loops important for computational tasks?
9. Briefly explain the role of the `SELECT CASE` statement in FORTRAN programs.
10. How does the Linux `nano` editor help in writing and editing FORTRAN code?

Category 2: Mid-Level (Understanding-Based)

1. Compare and contrast FORTRAN's built-in file-handling features with those in other programming languages.
2. Write a FORTRAN code snippet that reads two real numbers from a file and prints their sum.
3. How does FORTRAN's array indexing differ from Python's? What advantages does this provide in scientific computing?
4. Write a program to determine whether a given integer is even or odd using FORTRAN.
5. Describe how you would use FORTRAN to simulate the temperature distribution in a rod (hint: use arrays).
6. Explain how LAPACK can be used to solve a set of linear equations in FORTRAN. Why is linking external libraries beneficial?
7. Design a FORTRAN program to compute the factorial of a number using recursion.
8. How would you modify a FORTRAN program to store the computed results in a text file? Provide a pseudocode outline.

9. Describe how you would debug a FORTRAN program using Linux tools like `gdb` or compiler flags.
10. Explain the role of logical operators in FORTRAN with an example of their use in a physical simulation.

Category 3: Application-Based (Flowchart and Coding for Physics)

1. Write the algorithm and draw a flowchart to compute the determinant of a 3x3 matrix. Implement it in FORTRAN.
2. Create a flowchart and write a FORTRAN program to compute the trajectory of a projectile given its initial velocity and angle.
3. Develop an algorithm and flowchart for simulating the motion of a harmonic oscillator using Euler's method.
4. Create a flowchart and program in FORTRAN to calculate the area under a curve using the trapezoidal rule.
5. Write an algorithm and create a flowchart to compute the orbital velocity of a planet given its distance from the Sun. Implement the solution in FORTRAN.
6. Create a flowchart and write a FORTRAN program to solve the one-dimensional heat equation using finite differences.
7. Design a flowchart and write FORTRAN code to compute the discrete Fourier transform of a signal.
8. Write an algorithm and create a flowchart for calculating the electric field at a point due to multiple charges in 2D space.
9. Create a flowchart and program in FORTRAN to simulate a 2D random walk for a particle.
10. Write an algorithm and flowchart to calculate the energy levels of an electron in a one-dimensional potential well using the Schrödinger equation.

Chapter 2

Introduction to C++

C++ is a general-purpose programming language created as an extension of C by Bjarne Stroustrup in the early 1980s. It supports both procedural and object-oriented programming paradigms, making it versatile for systems programming, game development, and real-time applications.

2.1 Basic Syntax

C++ programs consist of statements that are grouped into functions and classes. The main function, `int main()`, is the starting point of any C++ program. Statements in C++ are terminated by semicolons, and the language is case-sensitive.

2.2 Variables and Data Types

C++ supports several basic data types, such as integers (`int`), floating-point numbers (`float`, `double`), characters (`char`), and booleans (`bool`). Variables are declared by specifying the type followed by the variable name.

2.3 Control Structures

C++ provides control structures like `if-else`, `switch-case`, loops (`for`, `while`, and `do-while`), and `goto` statements for controlling the flow of the program.

2.4 Functions

Functions in C++ allow for code reuse and modularization. A function is defined by specifying a return type, a name, and a list of parameters. The function body is enclosed in curly braces {}.

2.5 Arrays and Vectors

Arrays in C++ are a collection of elements of the same type. They are declared with a fixed size and can be single or multi-dimensional. Vectors, from the Standard Template Library (STL), offer dynamic sizing and more flexibility than arrays.

2.6 Object-Oriented Programming (OOP)

C++ is known for its support of object-oriented programming. It introduces the concepts of classes and objects, inheritance, polymorphism, encapsulation, and abstraction, which allow for modeling real-world entities in a more intuitive way.

2.7 File Handling

C++ provides file handling mechanisms through the `fstream` library. You can read from and write to files using `ifstream` (input file stream) and `ofstream` (output file stream).

2.8 Advanced Topics

Advanced features of C++ include templates, exception handling, operator overloading, and the Standard Template Library (STL) for generic programming. These features provide flexibility and efficiency in coding.

2.9 Example Programs

2.9.1 Basic syntax

```cpp
#include <iostream>
using namespace std;

int main() {
    cout << "Hello, World!" << endl;
    return 0;
}
```

To compile the program, use the following commands:

```
$ g++ hello.cpp -o hello
```

To run the compiled program, use:

```
$ ./hello
```

Output:

```
Hello, World!
```

2.9.2 Variables and data types

```cpp
#include <iostream>
using namespace std;

int main() {
    int i = 10;
    float f = 3.14;
```

```
    char c = 'A';
    bool b = true;

    cout << "Integer: " << i << endl;
    cout << "Float: " << f << endl;
    cout << "Character: " << c << endl;
    cout << "Boolean: " << b << endl;

    return 0;
}
```

To compile the program, use the following commands:

```
$ g++ variables.cpp -o variables
```

To run the compiled program, use:

```
$ ./variables
```

Output:

```
Integer: 10
Float: 3.14
Character: A
Boolean: 1
```

2.9.3 Control structures

```
#include <iostream>
using namespace std;

int main() {
    int i = 5;

    if (i > 0) {
        cout << "Positive" << endl;
    } else {
        cout << "Negative" << endl;
    }

    for (int j = 1; j <= 5; j++) {
        cout << j << endl;
    }
    return 0;
}
```

To compile the program, use the following commands:

```
$ g++ control.cpp -o control
```

To run the compiled program, use:

```
$ ./control
```

Output:

```
Positive
1
2
3
4
5
```

switch case:

```
#include <iostream>
using namespace std;

int main() {
    int i = 5;

    switch(i) {
        case 1:
            cout << "One" << endl;
            break;
        case 2:
            cout << "Two" << endl;
            break;
        default:
            cout << "Other" << endl;
    }

    return 0;
}
```

To compile the program, use the following commands:

```
$ g++ control_1.cpp -o control_1
```

To run the compiled program, use:

```
$ ./control_1
```

Output:

```
Other
```

2.9.4 Arrays and vectors

```
#include <iostream>
#include <vector>
using namespace std;

int main() {
    int arr[3] = {1, 2, 3};
    vector<int> vec = {1, 2, 3, 4};
```

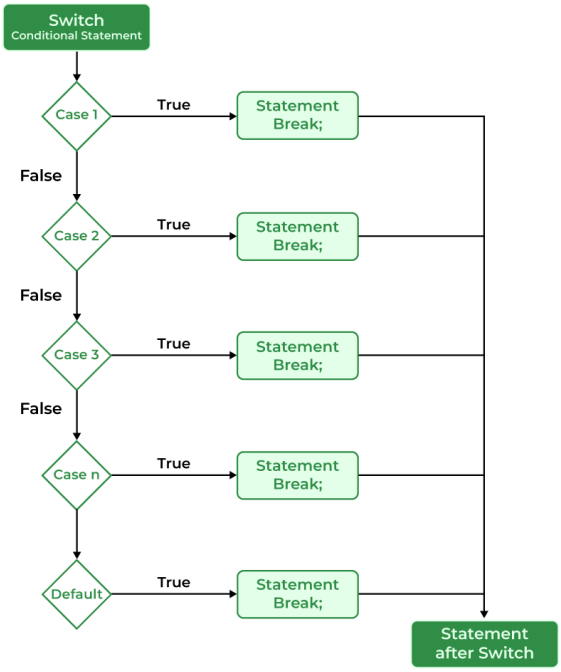


Figure 2.1: Switch case statements

```
8
9       cout << "Array elements: ";
10      for (int i = 0; i < 3; i++) {
11          cout << arr[i] << " ";
12      }
13      cout << endl;
14
15      cout << "Vector elements: ";
16      for (int i = 0; i < vec.size(); i++) {
17          cout << vec[i] << " ";
18      }
19      cout << endl;
20
21      return 0;
22  }
```

To compile the program, use the following commands:

```
1  $ g++ arrays.cpp -o arrays
```

To run the compiled program, use:

```
1  $ ./arrays
```

Output:

```
1  Array elements: 1 2 3
2  Vector elements: 1 2 3 4
```


2.9.5 Functions

```cpp
#include <iostream>
using namespace std;

int add(int a, int b) {
    return a + b;
}

int main() {
    int x = 5, y = 10;
    int sum = add(x, y);
    cout << "Sum: " << sum << endl;
    return 0;
}
```

To compile the program, use the following commands:

```
$ g++ functions.cpp -o functions
```

To run the compiled program, use:

```
$ ./functions
```

Output:

```
Sum: 15
```

2.9.6 File handling

```cpp
// C++ Program to Read a File Line by Line using ifstream
#include <fstream>
#include <iostream>
#include <string>

using namespace std;

int main()
{
    // Open the file "abc.txt" for reading
    ifstream inputFile("abc.txt");

    // Variable to store each line from the file
    string line;

    // Read each line from the file and print it
    while (getline(inputFile, line)) {
        // Process each line as needed
        cout << line << endl;
    }

    // Always close the file when done
```

```
    inputFile.close();

    return 0;
}
```

To compile the program, use the following commands:

```
$ g++ file_handling.cpp -o file_handling
```

To run the compiled program, use:

```
$ ./file_handling
```

The example program to write into a file in C++ using 'ofstream':

```
#include <iostream>
#include <fstream>  // Required for file handling
using namespace std;

int main() {
    // Declare an output file stream (ofstream) object
    ofstream outputFile;

    // Open a file named "example.txt"
    outputFile.open("example.txt");

    // Check if the file opened successfully
    if (!outputFile) {
        cout << "Error opening file!" << endl;
        return 1;  // Exit the program with an error code
    }

    // Write data to the file
    outputFile << "This is a simple example of writing to a file
   in C++.\n";
    outputFile << "File handling is important for many
   applications.\n";
    outputFile << "Learning how to write and read files is
   essential!\n";

    // Close the file
    outputFile.close();

    // Notify the user
    cout << "Data successfully written to the file!" << endl;

    return 0;
}
```

2.10 Pointers in C++

A pointer in C++ is a variable that stores the memory address of another variable. Pointers are widely used in C++ for dynamic memory management, passing parameters

by reference, and for working with arrays and data structures.

The syntax for declaring a pointer is:

```
type* pointer_name = &var_name;
```

Here, type refers to the data type that the pointer will point to.
Key operations with pointers:

- **Address-of operator** (`&`): Used to get the address of a variable.
- **Dereference operator** (`*`): Used to access the value stored at the address the pointer holds.

2.10.1 Examples

```
// Example 1: Basic pointer usage
#include <iostream>
using namespace std;

int main() {
    int var = 10;
    int* ptr = &var;  // Pointer to var

    cout << "Value of var: " << var << endl;
    cout << "Address of var: " << &var << endl;
    cout << "Value stored in ptr (address of var): " << ptr << endl;
    cout << "Dereferencing ptr to get value of var: " << *ptr << endl;

    return 0;
}
```

2.11 Arrays in C++

An array in C++ is a collection of elements of the same data type, stored in contiguous memory locations. Arrays can be accessed using index values starting from 0.

The syntax for declaring an array is:

```
type array_name[size] = {_, _, ...};
```

Important properties of arrays:

- Arrays can store multiple values in a single variable.
- The elements in an array are stored in contiguous memory locations.
- Arrays can be passed to functions by reference, meaning the memory address of the first element is passed.

2.11.1 Examples

```cpp
// Example 2: Working with arrays
#include <iostream>
using namespace std;

int main() {
    int arr[5] = {1, 2, 3, 4, 5};

    // Accessing array elements using indices
    cout << "First element: " << arr[0] << endl;
    cout << "Third element: " << arr[2] << endl;

    // Using a loop to print all elements
    for(int i = 0; i < 5; i++) {
        cout << "Element at index " << i << ": " << arr[i] << endl;
    }

    return 0;
}
```

2.12 Pointers and Arrays

In C++, arrays and pointers are closely related. The name of an array acts as a pointer to the first element of the array. This allows for pointer arithmetic and manipulation of array elements via pointers.

2.12.1 Examples

```cpp
// Example 3: Pointers and arrays
#include <iostream>
using namespace std;

int main() {
    int arr[3] = {10, 20, 30};
    int* ptr = arr;  // ptr points to the first element of the array

    // Accessing array elements via pointer
    for (int i = 0; i < 3; i++) {
        cout << "Element " << i << ": " << arr[i] << endl;
        cout << "Element " << i << ": " << *(ptr + i) << endl;
    }

    return 0;
}
```

2.13 Dynamic list Example

In this example, we need to manage the scores of a class of students. Since the number of students is unknown at compile-time, we will use dynamic memory allocation to create an array to store their scores at runtime. This demonstrates how pointers are used in dynamic memory management.

```
// Example: Managing a dynamic list of student scores
#include <iostream>
using namespace std;

int main() {
    int numStudents;

    // Asking the user for the number of students
    cout << "Enter the number of students: ";
    cin >> numStudents;

    // Dynamically allocating an array to store student scores
    float* scores = new float[numStudents];

    // Taking input for student scores
    for(int i = 0; i < numStudents; ++i) {
        cout << "Enter score for student " << i+1 << ": ";
        cin >> scores[i];
    }

    // Calculating the average score
    float sum = 0;
    for(int i = 0; i < numStudents; ++i) {
        sum += scores[i];
    }
    float average = sum / numStudents;

    // Displaying the average score
    cout << "Average score: " << average << endl;

    // Freeing the dynamically allocated memory
    delete[] scores;

    return 0;
}
```

2.13.1 Explanation

In this program, the number of students is provided by the user at runtime. The program dynamically allocates memory for the student scores using a pointer. The key steps are as follows:

- **Dynamic Memory Allocation**: `new float[numStudents]` allocates memory for an array of floats based on the number of students entered by the user. This is useful

when the size of data is not known during compile-time.

- **Pointer Usage**: The pointer `scores` stores the address of the first element of the dynamically allocated array. The notation `scores[i]` is used to access the array elements. This is equivalent to `*(scores + i)`, where pointer arithmetic is applied to traverse the memory.
- **Memory Deallocation**: The program uses `delete[]` to free the dynamically allocated memory after it is no longer needed, preventing memory leaks.

2.14 Significance of Using Pointers

Pointers in C++ are crucial for dynamic memory management, which provides several benefits in real-world applications:

- **Efficient Memory Usage**: Pointers allow for dynamic allocation of memory, meaning we can allocate memory based on actual needs at runtime. This avoids wastage of memory that occurs when arrays are declared with a fixed size at compile-time.
- **Flexibility**: Since the size of the array is determined at runtime, the program can handle variable amounts of data. This is particularly important when dealing with user input or data that fluctuates during program execution.
- **Performance**: Pointers can directly access and manipulate memory, making them more efficient in scenarios where performance is critical, such as handling large datasets, network buffers, or game engines.
- **Dynamic Data Structures**: Many advanced data structures like linked lists, trees, and graphs rely on pointers to manage memory and relationships between elements. These structures are widely used in algorithm design and systems programming.

Exercise

Category 1: Easy (Conceptual and Memory-Based)

1. What are the main features of C++ that make it suitable for systems programming and real-time applications?
2. Briefly explain the difference between procedural programming and object-oriented programming.
3. What is the purpose of the `int main()` function in a C++ program?
4. List the basic data types in C++ and provide an example of how to declare each.
5. What is the significance of the `#include` directive in C++?
6. Why is the semicolon (`;`) important in C++? Provide an example of its usage.
7. What is the difference between an array and a vector in C++?
8. Describe the role of the Standard Template Library (STL) in C++.
9. What are the key features of object-oriented programming supported by C++?
10. Explain the importance of the `fstream` library in C++ file handling.

Category 2: Mid-Level (Understanding-Based)

1. Write a simple C++ program to print the Fibonacci sequence up to `n` terms, where `n` is input by the user.
2. Describe how a `switch-case` statement works in C++. Provide an example of its usage.
3. Compare and contrast `for`, `while`, and `do-while` loops in C++.
4. Write a C++ function to calculate the factorial of a number using recursion.
5. How do pointers work in C++? Write a program to demonstrate the use of pointers to access and modify an integer variable.
6. Explain how to dynamically allocate and deallocate memory for an array in C++ using pointers.
7. Describe the difference between `ifstream` and `ofstream`. Provide an example of each.
8. Write a program to demonstrate the usage of vectors in C++ for storing and manipulating a list of integers.
9. How does operator overloading work in C++? Write a program to overload the `+` operator for adding two complex numbers.
10. Explain the use of templates in C++ with an example of a function template for swapping two variables.

Category 3: Application-Based (Flowchart and Coding)

1. Write the algorithm and draw a flowchart to compute the roots of a quadratic equation using the quadratic formula. Implement it in C++.
2. Create a flowchart and write a program to simulate the motion of a pendulum using simple harmonic motion equations.
3. Develop an algorithm and flowchart to compute the dot product of two vectors. Implement the solution in C++.
4. Create a flowchart and program to simulate the motion of a projectile given initial velocity and angle of projection.
5. Write a program to solve a system of linear equations using matrices and Gaussian elimination. Provide the algorithm and flowchart.
6. Develop an algorithm and flowchart to compute the numerical integration of a function using Simpson's rule. Write the corresponding C++ code.
7. Write the algorithm and create a flowchart to calculate the electric field at a point due to multiple charges in 2D space. Implement it in C++.
8. Design a flowchart and write a C++ program to simulate a simple 2D random walk of a particle.
9. Create an algorithm and flowchart for managing a dynamic list of student scores, including input, average calculation, and memory deallocation. Implement it in C++.
10. Write an algorithm and flowchart for generating the first `n` terms of a geometric progression, then implement the program in C++.

Chapter 3

Introduction to Gnuplot

3.1 Overview

Gnuplot is a portable command-line driven graphing utility for visualizing mathematical functions and data. It supports various types of plots in both 2D and 3D and can output to multiple formats, including PNG, PDF, SVG, and LaTeX. Gnuplot is widely used for its flexibility and ability to produce publication-quality graphics.

3.2 Getting Started with Gnuplot

To begin using Gnuplot, ensure it is installed on your system. You can download it from the official website: http://www.gnuplot.info/. After installation, launch the Gnuplot command-line interface by typing `gnuplot` in your terminal.

3.3 Plotting Mathematical Functions

Gnuplot allows for straightforward plotting of mathematical functions. For example, to plot the sine function:

```
gnuplot> plot sin(x)
```

This command will display a 2D plot of $\sin(x)$ over a default range. To specify a range for the x-axis:

```
gnuplot> plot [-10:10] sin(x)
```

3.4 Plotting Data from Files

Gnuplot can plot data from files where data is organized in columns. Consider a data file named `data.dat` with the following content:

```
# X   Y
1   2
2   4
3   6
4   8
```

```
5   10
```

To plot this data:

```
gnuplot> plot 'data.dat' using 1:2 with linespoints
```

This command tells Gnuplot to plot the first column as the x-axis and the second column as the y-axis, using lines and points to represent the data.

3.5 Customizing Plots

Gnuplot offers various customization options:

- **Titles and Labels** Add titles and axis labels to your plot.

```
gnuplot> set title "Sample Data Plot"
gnuplot> set xlabel "X-axis"
gnuplot> set ylabel "Y-axis"

```

- **Grid and Key (Legend)** Enable grid lines and position the legend.

```
gnuplot> set grid
gnuplot> set key right top

```

- **Output to Files** Save plots to files in various formats.

```
gnuplot> set terminal png
gnuplot> set output 'plot.png'
gnuplot> replot
gnuplot> set output

```

3.6 Examples

Example 1: Plotting Multiple Functions

To plot multiple functions on the same graph:

```
gnuplot> plot sin(x) title `sin(x)`, cos(x) title `cos(x)'
```

This command plots both $\sin(x)$ and $\cos(x)$ with respective titles.

Example 2: 3D Plotting

Gnuplot can create 3D plots using the `splot` command:

```
gnuplot> set hidden3d
gnuplot> splot sin(x)*cos(y) title `sin(x)cos(y)'
```

This will render a 3D surface plot of the function $\sin(x)\cos(y)$.

Example 3: Plotting Data with Error Bars

If your data file `data_with_errors.dat` includes errors:

```
# X   Y   Y_Error
1   2   0.1
2   4   0.2
3   6   0.1
4   8   0.3
5  10   0.2
```

Plot with error bars using:

```
gnuplot> plot "data_with_errors.dat" using 1:2:3 with yerrorbars
```

This command plots the data points with vertical error bars.

Exercises

Category 1: Easy (Conceptual and Memory-Based)

1. What is Gnuplot, and what are its primary uses?
2. List three types of plots that Gnuplot can generate.
3. How can you set the title of a plot in Gnuplot?
4. Describe the purpose of the `set xlabel` and `set ylabel` commands.
5. What command is used to plot a mathematical function in Gnuplot?

Category 2: Mid-Level (Understanding-Based)

1. Explain how to plot data from a file in Gnuplot. What does the `using` keyword specify?
2. How can you customize the range of the x-axis and y-axis in a plot?
3. Describe the steps to save a plot as a PNG file.
4. What is the difference between the `plot` and `splot` commands?
5. How can you add a legend to your plot, and where can it be positioned?

Category 3: Application-Based

1. Create a Gnuplot script to plot the function $f(x) = e^{-x^2}$ over the range $[-2 : 2]$.
2. Given a data file `experiment.dat` with three columns (time, measurement, error), write a Gnuplot command to plot the measurements with error bars.
3. Write a Gnuplot script to generate a 3D surface plot of $z = \sin(x) \times \cos(y)$.
4. How would you modify the appearance of the plot to use lines instead of points for data visualization?
5. Develop a Gnuplot script to plot multiple datasets from different files on the same graph, each with a distinct style and title.

Chapter 4

Introduction to LaTeX

4.1 Introduction to LaTeX

LaTeX is a powerful typesetting system extensively used in academia, especially for scientific documents that involve complex mathematical equations, figures, and references. It allows users to focus on the content while managing the formatting and layout efficiently. Unlike WYSIWYG (what you see is what you get) editors like Microsoft Word, LaTeX operates using plain text markup, which means you define structure and style using commands.

Key features of LaTeX include:

- Precise control over document formatting.
- Easy management of bibliographies, references, and citations.
- Automatic numbering and cross-referencing.
- Superior handling of mathematical formulas.

This document will guide you through the basics of LaTeX and demonstrate how to create well-structured documents with high-quality formatting.

4.2 Getting Started with LaTeX

4.2.1 Installing LaTeX

LaTeX is available on most platforms:

1. **Windows**: Use **MikTeX** or **TeX Live**.
2. **Mac**: Install **MacTeX**.
3. **Linux**: Install via package managers, e.g., `sudo apt-get install texlive-full`.

Popular editors:

- **TeXworks** (included with MikTeX).
- **Overleaf** (online collaborative LaTeX editor).
- **Texmaker** or **VS Code** with LaTeX plugins.

4.2.2 First LaTeX Document

A typical LaTeX document contains a preamble and a body. Below is an example of a basic document:

LaTeX Code:

```
\documentclass{article}
\usepackage[utf8]{inputenc}

\title{My First Document}
\author{John Doe}
\date{\today}

\begin{document}
\maketitle

Hello, this is my first
   document created with \
   LaTeX.
\end{document}

```

Output:

My First Document

John Doe

January 23, 2025

Hello, this is my first document created with LaTeX.

To compile this, run `pdflatex` and a PDF will be generated.

4.3 The Preamble and Body of a LaTeX Document

A LaTeX document consists of two main parts: the **preamble** and the **body**.

4.3.1 The Preamble

The preamble is the part of the document before the `\begin{document}` command. It is used to set up the overall structure and formatting of the document. Key components of the preamble include:

- `\documentclass{...}`: This command defines the type of document you are writing (e.g., `article`, `report`, `book`, etc.). You can also pass options to modify the appearance of the document, such as font size or paper size:

```
    \documentclass[12pt, a4paper]{article}

```

- `\usepackage{...}`: This command imports additional packages to enhance the functionality of your document. For example, to support UTF-8 character encoding or to add mathematical capabilities:

```
    \usepackage[utf8]{inputenc}
    \usepackage{amsmath}

```

- Title information commands:

- `\title{...}`: Sets the document title.
- `\author{...}`: Sets the author's name.
- `\date{...}`: Sets the date. You can use `\today` to automatically insert the current date.

These settings are later used when the `\maketitle` command is called in the body of the document.

4.3.2 The Body

The body of the document begins after the `\begin{document}` command. This is where the actual content of your document is written. You can include sections, text, lists, tables, figures, equations, and other elements. Here is an example of a simple document body:

```
\begin{document}
\maketitle

This is the body of the document. You can add sections like this:
\section{Introduction}
This is an introduction to my document.

You can also include mathematical equations, figures, and tables
   here.
\end{document}
```

The body ends with the `\end{document}` command, which signals the end of the document.

4.4 Document Structure

4.4.1 Basic Structure

A LaTeX document is organized using sections, subsections, and paragraphs. Here's a quick example:

LaTeX Code:

```
\section{Introduction}
This is the introduction.

\subsection{Background}
This is the background.

\subsubsection{Details}
Further details go here.

\paragraph{Note} This is a
   note.

```

Output:

1. Introduction

This is the introduction.

1.1 Background

This is the background.

1.1.1 Details

Further details go here.

Note This is a note.

4.4.2 Lists

Unordered List:

```
\begin{itemize}
    \item First item
    \item Second item
\end{itemize}
```

Output:

- First item
- Second item

Ordered List:

```
\begin{enumerate}
    \item First item
    \item Second item
\end{enumerate}
```

Output:

1. First item
2. Second item

4.5 Mathematical Typesetting

4.5.1 Inline Math

Inline math is simple to include. For example, the equation of a line can be written as follows:

```
The equation of a line is $y = mx + c$.
```

Output:

The equation of a line is $y = mx + c$.

4.5.2 Displayed Equations

For more complex math that needs its own line, use displayed math:

```

$$ E = mc^2 $$
```

Output:

$$E = mc^2$$

4.5.3 Complex Equations

Integrals can be written as:

```
$$ \int_a^b f(x) dx $$
```

Output:

$$\int_a^b f(x)dx$$

For more advanced math, use the `amsmath` package:

```
\documentclass{article}
\usepackage{amsmath}
% other packages in preamble

\begin{document}

% Your code


\end{document}
```

The `amsmath` package allows for advanced mathematical formatting. After including this package, you can use environments like `align`, `gather`, and more.

Complex Equations Using the `align` Environment

`align`: The `align` environment is used for aligning equations at the equal sign or other relation symbols:

LaTeX Code:

```
\begin{align}
    \int_0^{\infty} e^{-x} \, dx &= 1 \\
    \frac{d}{dx}(x^2) &= 2x \\
    \lim_{x \to 0} \frac{\sin x}{x} &= 1 \\
    e^{i\pi} + 1 &= 0
\end{align}
```

Output:

$$\int_0^{\infty} e^{-x}\,dx = 1 \tag{4.1}$$

$$\frac{d}{dx}(x^2) = 2x \tag{4.2}$$

$$\lim_{x\to 0} \frac{\sin x}{x} = 1 \tag{4.3}$$

$$e^{i\pi} + 1 = 0 \tag{4.4}$$

Complex Equations Using the `gather` Environment

The following equations include integrals, differentiation, and other mathematical symbols:

```
\begin{gather}
    \int_{a}^{b} f(x) \, dx = F(b) - F(a) \\
    \frac{d^2y}{dx^2} + p\frac{dy}{dx} + qy = 0 \\
    \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} \\
    \sqrt{a^2 + b^2} = c
\end{gather}
```

Output:

$$\int_a^b f(x)\,dx = F(b) - F(a) \tag{4.5}$$

$$\frac{d^2y}{dx^2} + p\frac{dy}{dx} + qy = 0 \tag{4.6}$$

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} \tag{4.7}$$

$$\sqrt{a^2 + b^2} = c \tag{4.8}$$

4.6 Figures and Tables

4.6.1 Inserting Figures

To include images in your LaTeX document, you need to use the `graphicx` package, which provides commands for handling graphics and images.

Include the `graphicx` Package

First, ensure you have the following line in the preamble of your document:

```
\usepackage{graphicx}
```

Inserting a Figure

To insert a figure, you use the `figure` environment. Below is the basic syntax:

```
\begin{figure}[h!]
    \centering
    \includegraphics[width=0.75\textwidth]{image.png}
    \caption{Sample Image}
    \label{fig:image1}
\end{figure}
```

- **Figure Environment**: The `figure` environment is a floating container for figures, which allows LaTeX to place the figure at an optimal location in the document. The

optional argument `[h!]` suggests that LaTeX should place the figure "here," but it can be overridden to maintain document flow.

- `\centering`: This command centers the figure within the figure environment.
- `\includegraphics`: This command is used to include the actual image file. The `width` parameter can be specified as a relative value (e.g., `0.75\textwidth` to make the image three quarter the width of the text area) or as an absolute dimension.
- `\caption`: This command provides a caption for the figure that appears below the image, helping to explain or describe it.
- `\label`: This command creates a reference label for the figure, allowing you to refer to it elsewhere in your document using `\ref{fig:image1}`.

Output:

Figure 4.1: UPES

We can refer Figure 4.1 anywhere in the document using it's label.

Important Notes

- Make sure that the image file (e.g., `image.png`) is in the same directory as your `.tex` file for it to be displayed correctly.
- Adjust the `width` parameter as needed to fit your document layout.
- The `figure` environment allows LaTeX to manage the placement of the image, which might not always be exactly where you placed the code, depending on the surrounding content. Use placement options like `[h!]`, `[t]`, `[b]`, or combinations to suggest preferred placement.

4.6.2 Tables

Tables can be created using the `tabular` environment, which provides a flexible way to arrange data in rows and columns. The structure of a table is defined using a combination of alignment specifiers, formatting commands, and optional features.

Basic Structure

The basic structure of a table consists of the following components: - The `table` environment, which allows for the placement of the table in a floating manner. - The `tabular` environment, which defines the actual content of the table.

Here is an example of a simple table:

```
\begin{table}[h!]
    \centering
    \begin{tabular}{|c|c|c|}
        \hline
        A & B & C \\
        \hline
        1 & 2 & 3 \\
        4 & 5 & 6 \\
        \hline
    \end{tabular}
    \caption{Sample Table}
    \label{tab:table1}
\end{table}
```

Output:

A	B	C
1	2	3
4	5	6

Table 4.1: Sample Table

Components of the Table Example

- `table`[h!]: This environment wraps the table and allows it to float in the document. The optional argument `[h!]` suggests placing the table "here" if possible.
- `\centering`: Centers the table on the page.
- `tabular`{|c|c|c|}: This command defines the table structure. The | character adds vertical lines between the columns, and `c` denotes center alignment for each column. You can also use `l` for left alignment and `r` for right alignment.
- `\hline`: Inserts a horizontal line in the table, creating a clear separation between rows.
- `A & B & C` \\: This line specifies the first row of the table. The ampersand `&` separates the columns, and the double backslash \\ indicates the end of the row.
- `\caption{Sample Table}`: Provides a caption for the table that appears above or below the table, depending on the document class and settings.
- `\label{tab:table1}`: This command creates a reference label for the table, allowing you to refer to it elsewhere in the document using `\ref{tab:table1}`.

Customizing Tables

You can customize tables in several ways:

1. **Changing Column Widths**: You can adjust the width of columns using the `pwidth` specifier instead of `c`, `l`, or `r`. For example, `p3cm` sets a fixed width for a column:

```
    \begin{tabular}{|p{3cm}|p{3cm}|p{3cm}|}
    \hline
    Long text in a column & Another column & More text \\
    \hline
    \end{tabular}

```

Output:

Long text in a column	Another column	More text

Table 4.2: My Caption

2. **Merging Cells**: To merge cells horizontally, you can use the `\multirow` or `\multicolumn` commands from the `multirow` package. Example of merging two columns:

```
\usepackage{multirow} % IN PREAMBLE (BEFORE \begin{document})

    \begin{table}[!h]
        \centering
           \begin{tabular}{|c|c|}
            \hline
            \multicolumn{2}{|c|}{Merged Cell} \\
            \hline
            1 & 2 \\
            3 & 4 \\
            \hline
            \end{tabular}
        \caption{Merged cells table}
        \label{tab:my_label_2}
    \end{table}

```

Output:

Merged Cell	
1	2
3	4

Table 4.3: Merged cells table

3. **Adding Borders and Color**: You can enhance the appearance of tables using the `booktabs` package, which provides commands like `\toprule`, `\midrule`, and `\bottomrule` for cleaner horizontal lines:


```latex
\usepackage{booktabs} % IN PREAMBLE (BEFORE \begin{document})

   \begin{table}[!h]
        \centering
        \caption{Tables using booktabs.}
        \begin{tabular}{ccc}
             \toprule
             A & B & C \\
             \midrule
             1 & 2 & 3 \\
             4 & 5 & 6 \\
             \bottomrule
             \end{tabular}
        \label{tab:my_label_3}
   \end{table}


```

Output:

Table 4.4: Tables using booktabs.

A	B	C
1	2	3
4	5	6

Example of a More Complex Table

Here's a more complex example that includes merged cells and custom widths:

```latex
\begin{table}[h!]
\centering
    \begin{tabular}{|p{4cm}|p{4cm}|c|}
    \hline
    \multicolumn{2}{|c|}{Combined Columns} & Single Column \\
    \hline
    Item 1 & Item 2 & Item 3 \\
    \hline
    \end{tabular}
\caption{Complex Table Example}
\label{tab:complex_table}
\end{table}
```

Output:

Combined Columns		Single Column
Item 1	Item 2	Item 3

Table 4.5: Complex Table Example

4.7 Cross-referencing and Bibliography

LaTeX provides powerful tools for cross-referencing and managing bibliographies. These features are particularly useful in larger documents like academic papers, theses, or reports, where you often need to refer to figures, tables, sections, or external references.

4.7.1 Cross-referencing

Cross-referencing in LaTeX allows you to refer to sections, figures, tables, equations, and more, without hardcoding specific numbers. This way, if your document structure changes, all references update automatically.

To set up a cross-reference, you use the `\label` command to mark a specific element, and then use `\ref` or `\pageref` to refer back to that element.

Cross-referencing Sections

For referencing sections, you can place the `\label` command immediately after the section heading. Here's an example:

```
\section{Introduction}\label{sec:intro}

This is the introduction to the paper.

\section{Methodology}\label{sec:method}

As discussed in Section \ref{sec:intro}, the problem is defined
   ...
```

Expected Output
As discussed in Section 1, the problem is defined...

Here, `\ref{sec:intro}` automatically inserts the section number ("1" in this case) into the text. If the order of sections changes, the reference will update to reflect the new numbering.

Cross-referencing Figures and Tables

Cross-referencing is also helpful for figures and tables. Here's an example for referencing a figure:

```
\begin{figure}[h!]
    \centering
    \includegraphics[width=0.5\textwidth]{example-image}
    \caption{An example image.}
    \label{fig:image1}
\end{figure}

As shown in Figure \ref{fig:image1}, the result is clear.
```

Expected Output
As shown in Figure 1, the result is clear.

In this case, the \label command inside the figure environment allows you to reference it using \ref{fig:image1}. The output will insert the figure number ("1" in this case) automatically.

You can similarly cross-reference tables by labeling them within the table environment:

```
\begin{table}[h!]
    \centering
    \begin{tabular}{|c|c|}
        \hline
        Item & Description \\
        \hline
        A & Example A \\
        B & Example B \\
        \hline
    \end{tabular}
    \caption{Example Table.}
    \label{tab:example}
\end{table}

Table \ref{tab:example} shows the details of items.
```

Expected Output
Table 1 shows the details of items.

Cross-referencing Pages

To refer to the page where an element appears, use the \pageref command. This is useful for long documents where you want to direct readers to the exact page of a figure, table, or section:

```
Figure \ref{fig:image1} is found on page \pageref{fig:image1}.
```

Expected Output
Figure 1 is found on page 2.

This command inserts the page number of the referenced element.

4.7.2 Bibliography

LaTeX is widely used in academic writing due to its excellent citation and bibliography management. LaTeX works with tools like BibTeX and BibLaTeX to handle references efficiently. BibTeX allows you to manage and format bibliographic data separately, while BibLaTeX provides more flexibility and modern features.

Basic Bibliography Using BibTeX

To use BibTeX, create a '.bib' file containing your references. In the main LaTeX file, include the following commands to generate the bibliography:

```
\bibliographystyle{plain}
\bibliography{references}
```


Here, `plain` is the style of the bibliography, and `references` is the name of your bibliography file (e.g., `references.bib`).

Your `.bib` file might look like this:

```
@book{lamport1994latex,
  title={LaTeX: A Document Preparation System},
  author={Lamport, Leslie},
  year={1994},
  publisher={Addison-Wesley}
}

@article{knuth1984texbook,
  title={The TeXbook},
  author={Knuth, Donald},
  journal={Computers \& Typesetting},
  volume={A},
  year={1984},
  publisher={Addison-Wesley}
}
```

When compiling your document, BibTeX automatically formats and adds the references at the end of your document. Citations can be added using the `\cite` command:

```
According to \cite{lamport1994latex}, \LaTeX{} is a powerful tool
    for document preparation.
```

Expected Output

According to [1], LaTeX is a powerful tool for document preparation.

At the end of your document, BibTeX generates the bibliography:

References

[1] Lamport, Leslie. LaTeX: A Document Preparation System. Addison-Wesley, 1994.

[2] Knuth, Donald. The TeXbook. Addison-Wesley, 1984.

Bibliography Using BibLaTeX

BibLaTeX is an advanced package for managing citations and bibliographies. To use it, load the package and specify the backend (e.g., biber):

```
\usepackage[backend=biber,style=numeric]{biblatex}
\addbibresource{references.bib}
```

This setup allows for more flexible citation styles, including numeric, alphabetic, author-year, and more. You can then cite sources using the `\cite` command just like in BibTeX:

```
\cite{knuth1984texbook}
```

At the end of the document, print the bibliography using:

```
\printbibliography
```


Citation Styles

Both BibTeX and BibLaTeX offer various citation styles. Common ones include:

- `plain`: Simple numbered style.
- `alpha`: Citations are based on authors' initials and publication year.
- `ieeetr`: IEEE citation style, commonly used in technical and engineering fields.
- `apalike`: APA-style citations, widely used in social sciences.

For example, to use the APA-like citation style:

```
\bibliographystyle{apalike}
```

Or, with BibLaTeX:

```
\usepackage[style=apa]{biblatex}
```

These commands will automatically format your citations and bibliography according to the selected style.

4.8 Customizing LaTeX Documents

Customization in LaTeX allows you to modify the appearance of your document to meet various formatting requirements. In this section, we'll cover some essential aspects of page layout, fonts, and text styles, all of which can be easily adjusted to suit your needs.

4.8.1 Page Layout

The page layout in a LaTeX document, such as paper size, margins, and orientation, can be customized using the `geometry` package. This package provides flexibility in adjusting the dimensions of the page to fit specific formatting needs.

To change the paper size and margins, you can specify options directly when loading the `geometry` package. Here's an example for setting A4 paper size and 1-inch margins:

```
\usepackage[a4paper, margin=1in]{geometry}
```

Customizing Margins

You can also specify custom margins for different sides of the page. For example, to set a 2-inch top margin, 1-inch bottom margin, 1.5-inch left margin, and 1-inch right margin, use:

```
\usepackage[top=2in, bottom=1in, left=1.5in, right=1in]{geometry}
```

Changing Paper Size and Orientation

To change the paper size to legal (8.5 x 14 inches) and make it landscape oriented, you can modify the options as follows:

```
\usepackage[legalpaper, landscape, margin=1in]{geometry}
```

Output: The page will be oriented horizontally (landscape) on legal-sized paper with 1-inch margins.

These changes will apply globally across the entire document unless you specify otherwise.

4.8.2 Font and Style

Font customization in LaTeX is managed by various packages, such as `fontenc` for encoding and `inputenc` for character sets. Changing fonts and text styles can improve readability and give your document a personalized look.

Font Encoding

Using the `fontenc` package ensures that fonts are properly encoded. For example, to enable T1 encoding, which allows for proper hyphenation and accented characters, use:

```
\usepackage[T1]{fontenc}
```

T1 encoding is essential when working with European languages or documents requiring accented characters.

Changing Fonts

You can change the font family to one of LaTeX's default font families, such as `serif`, `sans-serif`, or `monospace`, using the following commands:

```
\renewcommand{\familydefault}{\sfdefault}  % Sans-serif as
    default
```

To use a specific font, such as the popular `Times New Roman`, you can load the corresponding package:

```
\usepackage{times}  % Times New Roman
```

Output:
The entire document's font will switch to Times New Roman.
Other common font packages include:

1. `helvet` for Helvetica (sans-serif)
2. `courier` for Courier (monospace)

Text Styles

In LaTeX, text styles such as bold, italic, and underlined text are easily applied using the following commands:

1. **Bold Text:** Use `\textbf{...}` to make text bold.


```
This is \textbf{bold text}.
```

Output:

This is **bold text**.

2. **Italic Text:** Use `\textit{...}` to italicize text.

```
  This is \textit{italic text}.

```

Output:

This is *italic text*.

3. **Underlined Text:** While LaTeX doesn't have a direct underline command, you can use the `ulem` package to underline text:

```
  \usepackage{ulem}
  This is \uline{underlined text}.

```

Output:

This is underlined text.

Alternatively, for a simpler underlining solution, you can use the `underline` command from standard LaTeX:

```
  This is \underline{underlined text}.

```

Customizing Font Sizes

Font size can be adjusted globally or locally within the document. To set the font size for the entire document, modify the document class as follows:

```
\documentclass[12pt]{article}
```

This will set the default font size to 12 points.
For local font size adjustments, use the following commands within the document:

- `\tiny`: Very small text
- `\scriptsize`: Smaller than small
- `\footnotesize`: Slightly larger than `scriptsize`
- `\small`: Small text
- `\large`: Slightly larger text
- `\Large`, `\LARGE`: Progressively larger text
- `\huge`, `\Huge`: Very large text

Example:

```
This is \tiny{tiny text}, and this is \Huge{huge text}.
```

Output:

This is tiny text, and this is huge text.

By combining these commands, you can customize the look and feel of your document, ensuring it matches specific formatting guidelines or personal preferences.

4.8.3 Color and Highlighting

In LaTeX, the `xcolor` package is commonly used to apply colors to text and other elements. You can highlight important sections, change font colors, and even define your own custom colors.

To load the `xcolor` package:

```
\usepackage{xcolor}
```

Changing Text Color

To change the color of specific text, use the `\textcolor` command. Here's an example that sets the text color to red:

```
This is \textcolor{red}{red text}.
```

Output:

This is red text.

Highlighting Text

You can also highlight text with a background color using the `\colorbox` command:

```
\colorbox{yellow}{This text is highlighted in yellow.}
```

Output:

This text is highlighted in yellow.

Customizing LaTeX documents provides a great deal of flexibility in terms of page layout, fonts, text styles, and colors. Using the `geometry` package, you can control the page dimensions and margins. Text appearance can be easily managed with font encodings, font family selection, and local style adjustments like bold, italics, and color. Together, these tools allow you to craft a professional and visually appealing document.

4.9 Error Handling and Debugging

When working with LaTeX, errors can arise during the compilation process. Understanding common error messages and how to resolve them is essential for smooth document preparation. LaTeX editors, such as Overleaf, TeXShop, or TeXworks, provide detailed logs that can help you trace and fix errors.

In this section, we'll look at common errors, their causes, and strategies for debugging.

4.9.1 Common LaTeX Errors

Here are some of the most common errors you might encounter when compiling a LaTeX document:

Missing or Mismatched Braces

One of the most frequent errors is missing or unmatched braces (i.e., {...}). Every opening brace { must have a corresponding closing brace }.

Example Error:

```
This is an \textbf{example of missing brace.
```

The error message may look like this:

```
! LaTeX Error: \textbf on input line 1 ended by \end{document}.
```

Solution: Ensure that every { has a matching }. The correct syntax is:

```
This is an \textbf{example of correct brace}.
```

If you're dealing with nested braces, carefully check that each pair is properly closed.

Undefined References

Undefined references occur when you try to reference a section, figure, table, or citation that has not been labeled correctly or is missing entirely. You will see a warning like this during compilation:

```
LaTeX Warning: There were undefined references.
```

Example Error:

```
As shown in Figure \ref{fig:missing}, the results are clear.
```

If no figure with the label `fig:missing` exists, you'll get an error.

Solution: Ensure that you have labeled the element you're referencing. For example:

```
\begin{figure}[h!]
    \includegraphics[width=0.5\textwidth]{example-image}
    \caption{An example image.}
    \label{fig:image1}
\end{figure}

As shown in Figure \ref{fig:image1}, the results are clear.
```

Also, make sure to run multiple compilation steps (e.g., in Overleaf, press "Recompile" twice) to resolve cross-references.

Package Errors

Using incorrect or incompatible packages can lead to compilation errors. This happens if a required package is missing from your LaTeX installation or if two packages conflict with each other.

Example Error: If you try to load a non-existent package:

```
\usepackage{nonexistent}
```

You will see an error message like this:

```
! LaTeX Error: File 'nonexistent.sty' not found.
```

Solution: Ensure that the package you're trying to use is installed or available in your LaTeX distribution. For example, replace it with a valid package:

```
\usepackage{graphicx}  % A valid package
```

For package conflicts, try commenting out one of the conflicting packages or look for a compatible alternative.

4.9.2 Debugging Tips

Here are some strategies to debug your LaTeX documents effectively:

Read the Log File

Most LaTeX editors provide a detailed log file that lists all warnings and errors encountered during compilation. This log can help pinpoint the exact line where the error occurred. The log will often include the following types of messages:

- **Error messages**: These are critical and stop the compilation.
- **Warnings**: These indicate potential issues but do not stop the compilation.
- **Overfull/Underfull boxes**: These warn about text that overflows or does not properly fit in the margins.

To view the log, look for the "Log" or "Compiler" section in your editor. In Overleaf, for instance, the log is displayed in a separate window after compilation.

Isolate the Problem

If you're facing a complex issue and cannot locate the source of the error, try commenting out large sections of your document. You can use the % symbol to comment out lines of text or code temporarily:

```
%\section{Introduction}
%This section is commented out to isolate the problem.
```

Once you've isolated the error, you can start uncommenting sections one by one to find the problematic code.

Check for Typos in Labels

Typographical errors in labels are a common cause of undefined references. Double-check that your labels are spelled correctly and match the references exactly. LaTeX is case-sensitive, so {`fig:image1`} and {`fig:Image1`} will be treated as different labels.

Run Multiple Compilation Passes

When using cross-references or bibliographies (especially with BibTeX or BibLaTeX), LaTeX often requires multiple compilation passes to resolve all references. You may need to run:

1. `pdflatex`
2. `bibtex`
3. `pdflatex` (twice more)

This ensures that all citations and references are updated correctly.

4.9.3 Warnings

While warnings do not stop compilation, they can indicate formatting problems or overlooked issues. Some common warnings include:

Overfull or Underfull Boxes

These occur when text exceeds the margins (overfull) or does not fill the available space properly (underfull). The message may look like this:

```
Overfull \hbox (5.0pt too wide) in paragraph at lines 22--23
```

Solution: Adjust the text, font size, or use the `\sloppy` command to relax the formatting rules.

Undefined Citations

If a citation is not defined in the bibliography, you'll see a warning like:

```
LaTeX Warning: Citation 'key' on page 3 undefined.
```

Solution: Ensure that the citation key matches the reference in your `.bib` file.

4.9.4 Tools for Error-Free LaTeX

Here are some tools and techniques that can help you avoid and fix errors in LaTeX documents:

Online Editors

Using online editors like Overleaf can make error handling easier since they offer real-time error messages and logs. Overleaf, for example, highlights errors and warnings as you type, making it easier to identify issues immediately.

`lacheck` and `chktex`

These are command-line tools designed to check LaTeX documents for common errors and potential formatting issues. `lacheck` checks the syntax of your document, while `chktex` focuses on typographical issues.

Error handling and debugging are crucial aspects of working with LaTeX. By understanding common errors, reading logs carefully, and using debugging strategies, you can efficiently resolve issues and ensure smooth compilation. With the right tools and techniques, error-free LaTeX documents are easy to achieve.

4.10 Title Page and Its Customization in LaTeX

The title page is the first page of a LaTeX document, serving as the cover for your work. It typically includes the title of the document, the author's name, the institution, the date, and sometimes additional information like the course name or the supervisor's name. Customizing the title page can help create a professional and polished look for your document.

4.10.1 Basic Title Page

To create a basic title page in LaTeX, you can use the `\title`, `\author`, and `\date` commands, followed by the `\maketitle` command. Here's a simple example:

```
\documentclass{article}

\title{The Title of Your Document}
\author{Your Name}
\date{\today}  % Automatically inserts today's date

\begin{document}

\maketitle  % Generates the title page

\end{document}
```

4.10.2 Customizing the Title Page

- **Changing Fonts and Sizes:** You can customize the font size and style of the title, author, and date by using font commands. For example:

```
\title{\huge \textbf{The Title of Your Document}}
\author{\Large Your Name}

```


- **Adding a Logo:** If you want to include a logo (e.g., your institution's logo), you can use the `graphicx` package:

```
\usepackage{graphicx}

\title{\includegraphics[width=0.5\textwidth]{logo.png}\\[1em]
    \Huge \textbf{The Title of Your Document}}

```

- **Customizing Layout:** To further customize the layout of the title page, you can create your own title page using the `titlepage` environment. This allows more flexibility in positioning elements:

```
\begin{titlepage}
    \centering
    \vspace*{2cm}  % Adds vertical space
    {\Huge \textbf{The Title of Your Document}}\\[1.5cm]
    {\Large Your Name}\\
    {\large Institution Name}\\
    {\large \today}\\[2cm]
    \includegraphics[width=0.3\textwidth]{logo.png}\\[1cm]
    {\large Course Name}\\
    {\large Supervisor Name}
    \vfill
\end{titlepage}

```

- **Using Packages:** You can also explore packages like `titling` or `fancyhdr` for more advanced customization of the title page and headers/footers.

4.10.3 Example of a Customized Title Page

Here's a complete example with a customized title page:

```
\documentclass{article}
\usepackage{graphicx}

\title{\huge \textbf{The Title of Your Document}}
\author{\Large Your Name}
\date{\today}

\begin{document}

\begin{titlepage}
    \centering
    \vspace*{2cm}
    \includegraphics[width=0.3\textwidth]{logo.png}\\[1.5cm]
    {\Huge \textbf{The Title of Your Document}}\\[1.5cm]
    {\Large Your Name}\\[0.5cm]
    {\large Institution Name}\\[1.5cm]
    {\large \today}\\[2cm]
    {\large Course Name}\\
```

```
    {\large Supervisor Name}
    \vfill
\end{titlepage}

\end{document}
```

Customizing the title page in LaTeX is straightforward, allowing you to create a visually appealing introduction to your document. With simple commands and environments, you can adjust the layout, include graphics, and modify text styles to match your preferences or institutional requirements.

Further Resources

- Overleaf LaTeX Documentation: https://www.overleaf.com/learn/latex/Main_Page
- CTAN (Comprehensive TeX Archive Network): https://ctan.org/

Exercise

Category 1: Easy (Conceptual and Memory-Based)

1. What is LaTeX, and how does it differ from WYSIWYG editors like Microsoft Word?
2. List three key features of LaTeX that make it popular for academic document preparation.
3. What is the purpose of the preamble in a LaTeX document?
4. Describe the function of the following commands in LaTeX: `\documentclass`, `\usepackage`, and `\maketitle`.
5. How can you include mathematical equations in a LaTeX document? Provide an example of an inline equation.
6. What are the differences between ordered and unordered lists in LaTeX? Write a simple example for each.
7. Why is the `graphicx` package used in LaTeX documents?
8. What are the basic components of a title page in LaTeX?
9. Explain the difference between `\section`, `\subsection`, and `\paragraph` in structuring a LaTeX document.
10. What is the advantage of using `\label` and `\ref` commands for cross-referencing in LaTeX?

Category 2: Mid-Level (Understanding-Based)

1. Write a simple LaTeX document that includes a title page with a title, author, date, and a centered image.
2. Describe how the `align` environment is used for complex equations in LaTeX. Provide an example.
3. How can you customize the margins of a LaTeX document? Write the command to set all margins to 1 inch.
4. Create a simple table using the `tabular` environment with three columns: Name, Age, and Country.
5. Explain the difference between `\textbf`, `\textit`, and `\underline`. Write an example showing their usage.
6. How can you handle errors like "undefined references" in a LaTeX document? Suggest debugging strategies.
7. Write a LaTeX code snippet to display the equation $E = mc^2$ as a standalone equation.

8. How can you include a bibliography in a LaTeX document? Provide the basic steps.
9. Explain how the `xcolor` package is used to change the color of text in LaTeX. Write an example to display text in red.
10. How can you dynamically create numbered references for figures and tables in LaTeX? Write a small example showing a labeled figure.

Category 3: Application-Based

1. Write a LaTeX document to include a centered image, a table, and a displayed equation.
2. Create a LaTeX document for a two-column article layout with separate sections for Introduction and Conclusion.
3. Write a LaTeX document with cross-references to figures, tables, and sections.
4. Insert and reference a figure in a LaTeX document. Provide the corresponding LaTeX code.
5. Write a LaTeX code snippet for creating a custom title page that includes a title, author name, date, course, and institution name.
6. Write a LaTeX document to demonstrate the use of inline, displayed, and complex equations (using the `amsmath` package).
7. Create a LaTeX document to manage multiple sections, each containing a figure, table, and equation.
8. Write a LaTeX document to generate a bibliography using BibTeX with at least two references.
9. Demonstrate how to use the `booktabs` package for creating professional-looking tables in LaTeX.
10. Write a LaTeX document with a custom page layout, including specific margin settings and page orientation.

Chapter 5

Finding Roots of an Equation

In this chapter, we will explore three fundamental numerical methods for finding roots of equations: the Bisection Method, the Secant Method, and Newton-Raphson Method. Each method will be introduced with theoretical concepts, illustrated with examples, and followed by practice questions to strengthen your understanding.

Introduction to Root-Finding Methods

Root-finding algorithms are essential in numerical analysis for solving equations of the form $f(x) = 0$. We will discuss three methods here:

- **Bisection Method** - a simple and reliable method.
- **Secant Method** - a faster approach that avoids calculating derivatives.
- **Newton-Raphson Method** - a powerful method using derivatives for rapid convergence.

5.1 Bisection Method

The Bisection Method is a numerical approach to find a root of a continuous function $f(x)$ within a specified interval. It is particularly useful when the function changes sign over an interval, indicating the presence of a root.

5.1.1 Method Explanation

The Bisection Method works as follows:

1. Choose an interval $[a, b]$ such that $f(a) \cdot f(b) < 0$. This guarantees that there is at least one root in $[a, b]$.
2. Calculate the midpoint $m = \frac{a+b}{2}$.
3. Evaluate $f(m)$. If $f(m) = 0$, then m is the root. Otherwise, update the interval as follows:
    - If $f(a) \cdot f(m) < 0$, set $b = m$.

- If $f(b) \cdot f(m) < 0$, set $a = m$.

4. Repeat the steps until the interval $[a, b]$ is sufficiently small, or until the midpoint m is accurate to the desired precision.

5.1.2 Example: Finding the Root of f(x) = sinx - x cosx

Let's find the root of the function $f(x) = \sin x - x\cos x$ in the interval $[4, 5]$ using the Bisection Method. We'll proceed step-by-step, calculating each midpoint and evaluating the function to see if we've narrowed down the root.

Initial Setup

$$f(x) = \sin x - x\cos x$$

Evaluating $f(x)$ at the endpoints:

$$f(4) = \sin(4) - 4\cos(4) \approx 1.8577719881465196$$

$$f(5) = \sin(5) - 5\cos(5) \approx -2.3772352019792695$$

Since $f(4) \cdot f(5) < 0$, there is a root between $x = 4$ and $x = 5$.

Iterative Steps

The following table shows the iterative steps for the Bisection Method applied to $f(x) = \sin x - x\cos x$ in the interval $[4, 5]$:

Iteration	a	b	$m = \frac{a+b}{2}$	$f(a)$	$f(b)$	$f(a) \cdot f(b)$	Interval Update
1	4	5	4.5	1.85777	-2.37724	-4.42 (< 0)	[4,5]
2	4	4.5	4.25	1.85777	-0.02895	-0.05 (< 0)	[4,4.5]
3	4.25	4.5	4.375	1.00088	-0.02895	-0.03 (< 0)	[4.25,4.5]
4	4.375	4.5	4.4375	0.50461	-0.02895	-0.01 (< 0)	[4.375,4.5]
5	4.4375	4.5	4.46875	0.24206	-0.02895	-0.01 (< 0)	[4.4375,4.5]
6	4.46875	4.5	4.484375	0.10756	-0.02895	-0.00 (< 0)	[4.46875,4.5]
7	4.484375	4.5	4.4921875	0.03955	-0.02895	-0.00 (< 0)	[4.484375,4.5]
8	4.4921875	4.5	4.49609375	0.00536	-0.02895	-0.00 (< 0)	[4.4921875,4.5]
9	4.4921875	4.49609375	4.494140625	0.00536	-0.01178	-0.00 (< 0)	[4.4921875,4.49609375]
10	4.4921875	4.494140625	4.4931640625	0.00536	-0.00321	-0.00 (< 0)	[4.4921875,4.494140625]
11	4.4931640625	4.494140625	4.49365234375	0.00108	-0.00321	-0.00 (< 0)	[4.4931640625,4.494140625]

Table 5.1: Bisection Method Iterations for $f(x) = \sin x - x\cos x$ in the interval $[4, 5]$

Final Answer

After continuing the iterations, we find that the root of $f(x) = \sin x - x\cos x$ to the desired precision in the interval $[4, 5]$ is approximately:

$$x \approx 4.49365234375$$

5.1.3 Error Estimation in the Bisection Method

In the Bisection Method, we iteratively narrow down the interval $[a, b]$ that contains the root. With each iteration, the interval's length is halved, allowing us to estimate the error and the convergence rate.

Absolute Error Bound

If we define the root as r, then after n iterations, the interval $[a_n, b_n]$ contains r. The error in the approximation $m_n = \frac{a_n+b_n}{2}$, which is the midpoint of the interval, is bounded by half the interval length:

$$|m_n - r| \leq \frac{b_n - a_n}{2} = \frac{b-a}{2^n}$$

where $[a, b]$ is the initial interval.

As n increases, the interval $[a_n, b_n]$ becomes smaller, leading to a smaller error bound. This error bound tells us how close our approximation m_n is to the actual root r.

Number of Iterations for Desired Accuracy

To achieve a specific accuracy ϵ, we can calculate the required number of iterations N as follows:

$$N \geq \log_2 \left(\frac{b-a}{\epsilon} \right)$$

This formula allows us to determine the minimum number of iterations needed to ensure that our approximation is within a specified tolerance ϵ from the true root.

Convergence Rate

The Bisection Method has a convergence rate of $\mathcal{O}(2^{-n})$, which means the error decreases by approximately half with each iteration. This linear convergence is slower compared to other methods like the Newton-Raphson Method, which has quadratic convergence, but the Bisection Method is more robust and guarantees convergence as long as the initial interval contains a root.

Example of Error Estimation

Suppose we start with an interval $[4, 5]$ and want to find the root of $f(x) = \sin x - x \cos x$ to within $\epsilon = 0.001$. Using the formula above, we can estimate the number of iterations needed:

$$N \geq \log_2 \left(\frac{5-4}{0.001} \right) = \log_2(1000) \approx 10$$

Therefore, at least 10 iterations are required to ensure that the error in our approximation is less than 0.001.

This error estimation helps us plan the number of iterations in advance and gives confidence that our final approximation is close to the true root within the desired accuracy.

5.1.4 Practice Questions

1. Use the Bisection Method to find the root of $f(x) = x^2 - 4$ on the interval $[0, 3]$ to three decimal places.

2. Apply the Bisection Method to find the root of $f(x) = \cos x - x$ on $[0, 1]$.

5.2 Secant Method

The Secant method is a numerical technique used to find the root of a function $f(x)$ by using a secant line to approximate the function near the root. Unlike the Bisection method, the two initial points for the Secant method do not need to lie on opposite sides of the root, but they must be sufficiently close to it. However, choosing points on opposite sides of the root often improves the stability of the method.

The Secant method uses two initial points, x_1 and x_2, and approximates the function by a straight line passing through these two points. The root is then estimated as the x-intercept of this secant line. The equation of the secant line passing through the points $(x_1, f(x_1))$ and $(x_2, f(x_2))$ is given by:

$$y - f(x_2) = \frac{f(x_2) - f(x_1)}{x_2 - x_1}(x - x_2)$$

Setting $y = 0$ to find the x-intercept (the approximation of the root), we get:

$$0 - f(x_2) = \frac{f(x_2) - f(x_1)}{x_2 - x_1}(x_3 - x_2)$$

Solving for x_3, the next approximation of the root is:

$$x_3 = x_2 - f(x_2)\frac{x_2 - x_1}{f(x_2) - f(x_1)}$$

This formula is iterated with the newly found point x_3 replacing x_1, and x_2 replacing x_3 in subsequent steps. The process is repeated until the values of x_n converge to a root with the desired level of accuracy.

5.2.1 Method Explanation

Given two points x_0 and x_1 close to the root, the secant method approximates the root using:

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

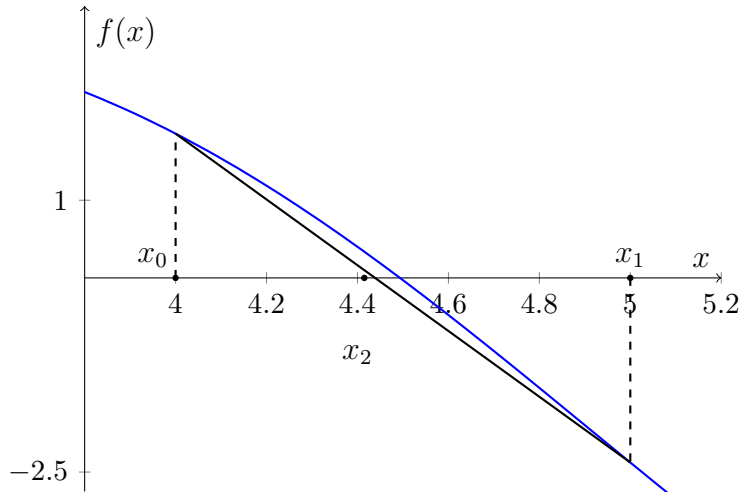


Figure 5.1: Secant method on f(x) = sin(x) - xcos(x).

5.2.2 Example: Solving $f(x) = \sin x - xcosx = 0$ for $x \in [4, 5]$

Let's apply the Secant Method to find the root of $f(x) = \sin x - x\cos x$ with x in radians and initial guesses $x_0 = 4.0$ and $x_1 = 5.0$. We will continue the iterations until the function value is close to zero, recording the process in a table.

$$f(x) = \sin x - x\cos x$$

Detailed Iterations in Table

Table 5.2: Solving $f(x) = \sin x - x\cos x$ using Secant method.

Iteration	x_n	x_{n-1}	$f(x_n)$	$x_{n+1} = x_n - f(x_n)\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}$
0	4.0	-	$f(4.0) = \sin(4.0) - 4.0\cos(4.0) \approx -2.613$	-
1	5.0	4.0	$f(5.0) = \sin(5.0) - 5.0\cos(5.0) \approx 3.418$	$x_2 = 4.0 - (-2.613)\frac{4.0-5.0}{-2.613-3.418} \approx 4.433$
2	4.433	5.0	$f(4.433) \approx -0.432$	$x_3 = 4.433 - (-0.432)\frac{4.433-5.0}{-0.432-3.418} \approx 4.490$
3	4.490	4.433	$f(4.490) \approx -0.030$	$x_4 = 4.490 - (-0.030)\frac{4.490-4.433}{-0.030+0.432} \approx 4.494$
4	4.494	4.490	$f(4.494) \approx 0.0005$	$x_5 = 4.494 - 0.0005\frac{4.494-4.490}{0.0005+0.030} \approx 4.4934$
5	4.4934	4.494	$f(4.4934) \approx 0$	Converged to root

Explanation of Iterations

In this table:
- **Iteration 0:** We start with initial guesses $x_0 = 4.0$ and $x_1 = 5.0$, calculating $f(x_0) \approx -2.613$ and $f(x_1) \approx 3.418$.
- **Iteration 1:** Using the Secant formula, we find $x_2 \approx 4.433$.
- **Iteration 2 to 4:** We continue the iterations, refining our approximations.
- **Iteration 5:** We reach $x \approx 4.4934$, where $f(x) \approx 0$, indicating the approximate root is $x \approx 4.4934$.

The Secant Method has successfully approximated the root of $f(x) = \sin x - x\cos x$ in the interval $[4, 5]$ to be around $x \approx 4.4934$. This iterative approach converges quickly and avoids the need for derivatives, making it a practical alternative to other root-finding methods.

5.2.3 Practice Questions

1. Find the root of $f(x) = x^2 - 2x + 1$ using the Secant Method with initial guesses $x_0 = 1.5$ and $x_1 = 2$.

2. Use the Secant Method to approximate the root of $f(x) = \sin x - 0.5$ with initial guesses $x_0 = 0.5$ and $x_1 = 1$.

5.3 Newton-Raphson Method

The Newton-Raphson Method uses the derivative to find a root of a function.

5.3.1 Method Explanation

Starting with an initial guess x_0, update x using:

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

5.3.2 Example

Find the root of $f(x) = x^3 - 3x + 2$ using Newton-Raphson with $x_0 = 0.5$.

5.3.3 Practice Questions

1. Use the Newton-Raphson Method to find the root of $f(x) = x^2 - 4x + 3$ starting with $x_0 = 2.5$.
2. Find the root of $f(x) = \tan(x) - x$ using an initial guess of $x_0 = 4$.

5.4 Summary and Comparison of Methods

In this chapter, we explored three methods of finding roots, each with unique advantages and limitations. Practice and apply these methods to determine which is best suited for a given problem.

Chapter 6

Interpolation

6.1 Lagrange Interpolation Formula

The **Lagrange Interpolation Formula** is used to find the polynomial $P(x)$ that passes through a given set of points $(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)$. It is given by:

$$P(x) = \sum_{i=0}^{n} y_i \cdot L_i(x),$$

where $L_i(x)$ is the Lagrange basis polynomial:

$$L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}.$$

Example

Problem: Find the interpolating polynomial using the points $(1, 1), (2, 4), (3, 9)$, and evaluate $P(2.5)$.

Step 1: Write the formula for $P(x)$

For three points, the polynomial is:

$$P(x) = y_0 \cdot L_0(x) + y_1 \cdot L_1(x) + y_2 \cdot L_2(x).$$

Step 2: Compute $L_0(x), L_1(x)$, and $L_2(x)$

$$\begin{aligned}
L_0(x) &= \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} = \frac{(x - 2)(x - 3)}{(1 - 2)(1 - 3)} = \frac{(x - 2)(x - 3)}{2}, \\
L_1(x) &= \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} = \frac{(x - 1)(x - 3)}{(2 - 1)(2 - 3)} = -\frac{(x - 1)(x - 3)}{1}, \\
L_2(x) &= \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} = \frac{(x - 1)(x - 2)}{(3 - 1)(3 - 2)} = \frac{(x - 1)(x - 2)}{2}.
\end{aligned}$$

Step 3: Substitute $y_0 = 1, y_1 = 4, y_2 = 9$ into $P(x)$

$$P(x) = 1 \cdot \frac{(x-2)(x-3)}{2} + 4 \cdot \left(-\frac{(x-1)(x-3)}{1}\right) + 9 \cdot \frac{(x-1)(x-2)}{2}.$$

Simplifying:

$$P(x) = \frac{(x-2)(x-3)}{2} - 4(x-1)(x-3) + \frac{9(x-1)(x-2)}{2}.$$

Step 4: Evaluate $P(2.5)$

Substitute $x = 2.5$:

$$L_0(2.5) = \frac{(2.5-2)(2.5-3)}{2} = \frac{(0.5)(-0.5)}{2} = -0.125,$$
$$L_1(2.5) = -\frac{(2.5-1)(2.5-3)}{1} = -(1.5)(-0.5) = 0.75,$$
$$L_2(2.5) = \frac{(2.5-1)(2.5-2)}{2} = \frac{(1.5)(0.5)}{2} = 0.375.$$

Now compute $P(2.5)$:

$$P(2.5) = 1(-0.125) + 4(0.75) + 9(0.375).$$

$$P(2.5) = -0.125 + 3 + 3.375 = 6.25.$$

Final Answer

The interpolated polynomial is:

$$P(x) = \frac{(x-2)(x-3)}{2} - 4(x-1)(x-3) + \frac{9(x-1)(x-2)}{2}.$$

At $x = 2.5$, $P(2.5) = 6.25$.

