

# Numerical Analysis for Chemical Engineers

Taechul Lee (tlee@prosys.korea.ac.kr)

---

- [Contents](#)
- [Modeling, Computers, and Error Analysis](#)
  - [Mathematical Modeling and Engineering Problem-Solving](#)
    - [A Simple Mathematical Model](#)
  - [Computers and Software](#)
    - [The Software Development Process](#)
    - [Algorithm Design](#)
    - [Program Composition](#)
    - [Quality Control](#)
  - [Approximations and Round-Off Errors](#)
    - [Significant Figures](#)
    - [Accuracy and Precision](#)
    - [Error Definitions](#)
  - [Truncation Errors and the Taylor Series](#)
    - [The Taylor Series](#)
    - [Using the Taylor Series to Estimate Truncation Errors](#)
    - [Numerical Differentiation](#)
- [Roots of Equations](#)
  - [Bracketing Methods](#)
    - [Graphical Methods](#)
    - [The Bisection Method](#)
    - [The False-Position Method](#)
  - [Open Methods](#)
    - [Simple Fixed-point Iteration](#)
    - [The Newton-Raphson Method](#)
    - [The Secant Method](#)
    - [Multiple Roots](#)
    - [Systems of Nonlinear Equations](#)
  - [Roots of Polynomials](#)
    - [Polynomials in Engineering and Science](#)
    - [Computing with Polynomials](#)
    - [Conventional Methods](#)
    - [Root Location with Libraries and Packages](#)
  - [Engineering Applications: Roots of Equations](#)
- [Linear Algebraic Equations](#)
  - [Gauss Elimination](#)
    - [Solving Small Numbers of Equations](#)
    - [Naive Gauss Elimination](#)
    - [Pitfalls of Elimination Methods](#)
    - [Techniques for Improving Solutions](#)
    - [Complex Systems](#)
    - [Nonlinear Systems of Equations](#)
    - [Gauss-Jordan](#)
  - [LU Decomposition and Matrix Inversion](#)
    - [LU Decomposition](#)
    - [The Matrix Inverse](#)
    - [Error Analysis and System Condition](#)
  - [Special Matrices and Gauss-Seidel](#)
    - [Special Matrices](#)
    - [Gauss-Seidel](#)
    - [Linear Algebraic Equation with Libraries and Packages](#)
  - [Engineering Applications: Linear Algebraic Equations](#)
- [Optimization](#)
  - [One-dimensional Unconstrained Optimization](#)
    - [Golden-Section Search](#)
    - [Quadratic Interpolation](#)

- Newton's Method
  - Multidimensional Unconstrained Optimization
    - Direct Methods
    - Gradient Methods
  - Constrained Optimization
    - Linear Programming
    - Optimization with Packages
  - Engineering Applications: Optimization
- Curve Fitting
  - Least-Squares Regression
    - Linear Regression
    - General Linear Least-Squares
    - Nonlinear Regression
  - Interpolation
    - Newton's Divided-Difference Interpolating Polynomials
    - Lagrange Interpolating Polynomial
    - Spline Interpolation
  - Fourier Approximation
    - Curve Fitting with Sinusoidal Functions
    - Fourier Integral and Transform
    - Discrete Fourier Transform (DFT)
    - Fast Fourier Transform (FFT)
    - The Power Spectrum
    - Curve Fitting with Libraries and Packages
  - Engineering Applications: Curve Fitting
- Numerical Differentiation and Integration
  - Newton-Cotes Integration of Equations
    - The Trapezoidal rule
    - Simpson's rule
  - Integrations of Equations
    - Romberg integration
    - Gauss Quadrature
    - Improper integrals
  - Numerical Differentiation
    - High-accuracy differentiation formulas
    - Richardson extrapolation
    - Derivatives of unequally spaced data
    - Numerical integration/differentiation formulas with libraries and packages
  - Engineering Applications: Numerical Integration and Differentiation
- Ordinary Differential Equations
  - Runge-Kutta Methods
    - Euler's Method
    - Improvement of Euler's Method
    - Runge-Kutta Method
    - Systems of Equations
    - Adaptive Runge-Kutta Method
  - Stiffness and Multistep Methods
    - Stiffness
    - Multistep Methods
  - Boundary-Value and Eigenvalue Problems
    - General Methods of Boundary-Value Problems
    - ODEs and Eigenvalues with Libraries and Packages
  - Engineering Applications: Ordinary Differential Equations
- Partial Differential Equations
  - Finite Difference: Elliptic Equations
    - The Laplace Equations
    - Solution Techniques
    - Boundary Conditions
    - The Control Volume Approach
  - Finite Difference: Parabolic Equations
    - The Heat Conduction Equation
    - Explicit Methods
    - A Simple Implicit Method
    - The Crank-Nicholson Method
  - Finite Element Method
    - Calculus of variation
    - Example: The shortest distance between two points
    - The Rayleigh-Ritz Method
    - The Collocation and Galerkin Method

- Finite elements for ordinary-differential equations
    - Engineering Applications: Partial Differential Equations
  - Using Matlab
    - 설치
    - Matlab 기초
      - 배열
      - Customization
      - Summary
    - 제어문
      - if, else, and elseif
      - switch
      - while
      - for
      - break
      - Summary
    - 함수만들기
    - Matlab에서 그림 그리기
      - plot 명령어
      - 고급 plot 명령어
      - 그림을 그리는 다른 명령어들
    - 예제
      - Linear Equation
  - Using Fortran
    - 설치 및 사용법
      - MS Window에서 작동하는 포트란
      - Unix 머신에서 작동하는 포트란
      - Summary
    - 데이터와 입출력
      - 기본적 구성
      - 기본적 데이터 타입
      - 입력과 출력에 관해
      - Redirection
      - Dimension
      - 데이터 초기화
      - Summary
    - 제어문
      - STOP문
      - GOTO문
      - PAUSE문
      - CONTINUE문
      - CALL문
      - RETURN문
      - IF문
      - DO문
      - Summary
    - 부프로그램
      - FUNCTION
      - SUBROUTINE
      - 부프로그램 컴파일
      - 라이브러리 만들기
      - EXTERNAL 문 사용하기
      - IMSL 사용하기
  - About this document ...

---

[Next](#)
[Up](#)
[Previous](#)
[Contents](#)

Next: Contents Up: HOME

Taechul Lee  
2001-11-29