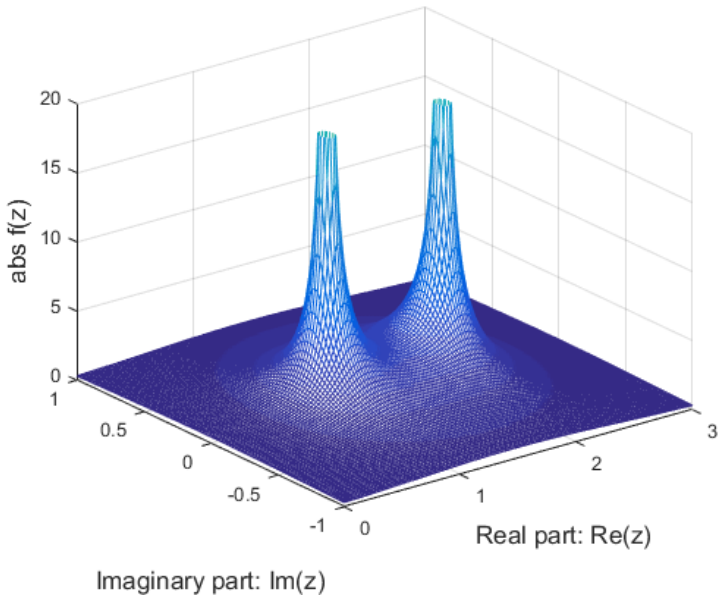
Report for Practice of Numerical Analysis

Spring 2025



Name:	Alif Zaicho Nur Ahmad 安曼迪
Student ID:	243519015
Subject:	Numerical Analysis
Email:	alifzaicho@csu.cn.edu
Source Code	github.com/alifzaicho/CSU-Numerical_Analysis_Spring_2025
School:	School of Metallurgy and Environment
University:	Central South University
Date:	May 19, 2025

Contents

1 Interpolation

1.1 Real Case: Interpolation of the normal distribution

In mineral processing, the feed grade (concentration of valuable mineral) of an ore varies with the particle size distribution (PSD). The PSD is modeled using a normal distribution:

$$f(x \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \tag{1}$$

where x is the particle size (in micrometers), μ is the mean size, and σ is the standard deviation.

1.2 General Polynomials

The monomial basis functions are defined as:

$$P_i(x) = x^i \tag{2}$$

A general polynomial of degree n is given by:

$$S_n(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n \tag{3}$$

The entries of the Hilbert matrix H are computed as inner products:

$$H_{i,j} = \int_a^b x^{i+j} dx = \frac{b^{i+j+1} - a^{i+j+1}}{i+j+1} \tag{4}$$

The entries of the d vector are computed as projections of $f(x)$ onto the basis functions:

$$d_i = \int_a^b f(x) x^i dx \tag{5}$$

The normal equations to solve are:

$$H \cdot \mathbf{a} = d \tag{6}$$

where H is the Hilbert matrix, $\mathbf{a}$ is the vector of coefficients to find, and d is the vector of projections.

1.2.1 Algorithm

Algorithm 1 Monomial Basis Approximation

Require: Function f, degree n, interval $[a, b]$
Ensure: Coefficients $\mathbf{a}$ for the monomial approximation
0: **Form the Hilbert matrix** H:
0: **for** $i = 0$ to n **do**
0: **for** $j = 0$ to n **do**
0: Compute inner product: $H[i][j] \leftarrow \int_a^b x^{i+j} dx$
0: This forms the Hilbert matrix with entries $H_{i,j} = \langle x^i, x^j \rangle$
0: **end for**
0: **end for**
0: **Construct the d vector**:
0: **for** $i = 0$ to n **do**
0: Compute projection: $d[i] \leftarrow \int_a^b f(x) x^i dx$
0: This forms the vector d with entries $d_i = \langle f(x), x^i \rangle$
0: **end for**
0: **Solve the normal equations**:
0: Solve the linear system $H \cdot \mathbf{a} = d$ for coefficients $\mathbf{a}$
0: **return a** =0

1.2.2 Python snippet for General polynomials

```python
import numpy as np
from scipy.integrate import quad

def monomial_interpolation(func, degree, lower=-1, upper=1):
    """
    Compute monomial interpolation coefficients for the given function.

    Args:
        func: Function to approximate
        degree: Degree of the interpolating polynomial
        lower: Lower bound of the interval
        upper: Upper bound of the interval

    Returns:
        coeff: Coefficients of the interpolating polynomial
    """
    # Build the matrix and right-hand side vector
    A = np.zeros((degree + 1, degree + 1))
    Y = np.zeros(degree + 1)

    for i in range(degree + 1):
        for j in range(degree + 1):
            integrand = lambda x: x**i * x**j
            A[i, j], _ = quad(integrand, lower, upper)
        integrand = lambda x: func(x) * x**i
        Y[i], _ = quad(integrand, lower, upper)
```

```
27
28      # Solve for coefficients
29      coeff = np.linalg.solve(A, Y)
30      return coeff
31
32  # Example usage:
33  def test_function(x):
34      return (1/np.sqrt(2*np.pi))*np.exp((-x**2)/2)
35
36  coefficients = monomial_interpolation(test_function, degree=3, lower=-1, upper=1)
37  print("Interpolation coefficients:", coefficients)
```

Listing 1: Monomial Interpolation

1.2.3 Results

The Hilbert matrix H for degree 6 is formed as follows:

$$H = \begin{bmatrix} 7 & 0 & 28.58 & 0 & 210.09 & 0 & 1838.27 \\ 0 & 28.58 & 0 & 210.09 & 0 & 1838.27 & 0 \\ 28.58 & 0 & 210.09 & 0 & 1838.27 & 0 & 17514.59 \\ 0 & 210.09 & 0 & 1838.27 & 0 & 17514.59 & 0 \\ 210.09 & 0 & 1838.27 & 0 & 17514.59 & 0 & 175543.92 \\ 0 & 1838.27 & 0 & 17514.59 & 0 & 175543.92 & 0 \\ 1838.27 & 0 & 17514.59 & 0 & 175543.92 & 0 & 1819580.27 \end{bmatrix}$$

The vector d is constructed as:

$$d^T = \begin{bmatrix} 1.00 & 0 & 0.99 & 0 & 2.91 & 0 & 13.61 \end{bmatrix}$$

The resulting coefficients are:

$$\mathbf{a}^T = \begin{bmatrix} 0.38 & 0 & -0.15 & 0 & 0.02 & 0 & 0.00 \end{bmatrix}$$

Using the resulting coefficients, the approximated polynomial is:

$$p(x) = 0.38 + (-0.15)x^2 + 0.02x^4 \tag{7}$$

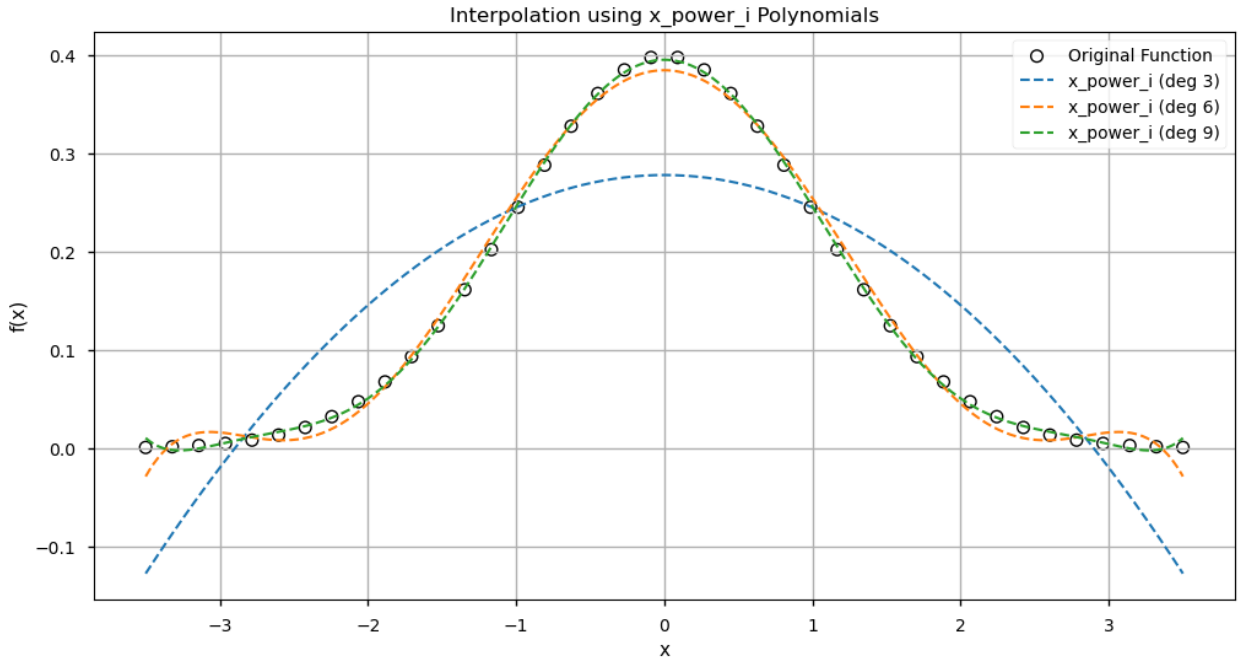


Figure 1: Interpolation method using general polynomials

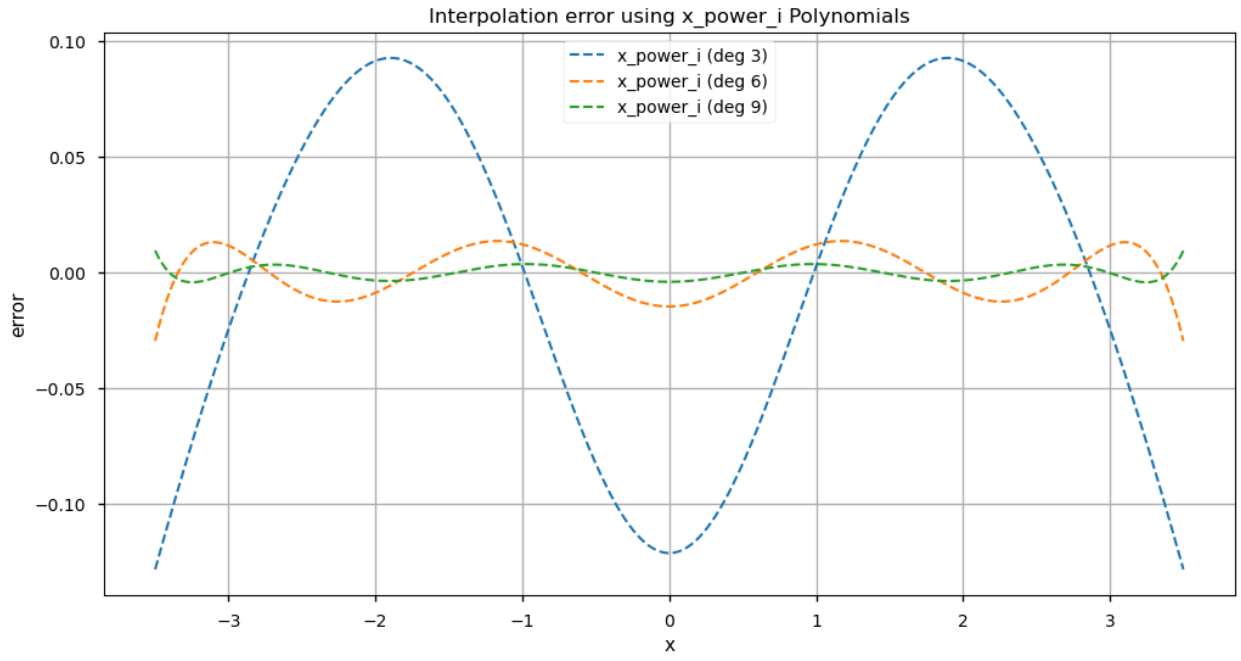


Figure 2: Interpolation error from general polynomials

1.2.4 Key Observations

- The Hilbert matrix H is symmetric and has a banded structure with alternating zero and non-zero entries.

- The vector d alternates between non-zero and zero values.
- The resulting coefficients $\mathbf{a}$ also alternate between non-zero and zero values, aligning with the structure of H and d.
- Even-indexed coefficients (0, 2, 4, 6) are non-zero, while odd-indexed coefficients (1, 3, 5) are zero.

1.3 Legendre Polynomials

The Legendre polynomials are defined as:

$$P_i(x) = \frac{1}{2^i i!} \frac{d^i}{dx^i} \left[(x^2 - 1)^i \right] \tag{8}$$

A general polynomial of degree n using Legendre polynomials is given by:

$$p_n(x) = a_0 P_0(x) + a_1 P_1(x) + a_2 P_2(x) + \cdots + a_n P_n(x) \tag{9}$$

The weight function for Legendre polynomials is typically 1, which simplifies the integration process. This is because Legendre polynomials are orthogonal over the interval $[-1, 1]$ with respect to the weight function $w(x) = 1$. The entries of the Hilbert matrix H for Legendre polynomials are computed as inner products:

$$H_{i,j} = \int_{-1}^{1} P_i(x) P_j(x) dx = \frac{2}{2i+1} \delta_{ij} \tag{10}$$

The entries of the d vector are computed as projections of $f(x)$ onto the Legendre polynomials:

$$d_i = \int_{-1}^{1} f(x) P_i(x) dx \tag{11}$$

The normal equations to solve are:

$$H \cdot \mathbf{a} = d \tag{12}$$

where H is the Hilbert matrix, $\mathbf{a}$ is the vector of coefficients to find, and d is the vector of projections.

1.3.1 Algorithm

Algorithm 2 Legendre Polynomial Approximation

Require: Function f, degree n, interval $[-1, 1]$
Ensure: Coefficients $\mathbf{a}$ for the Legendre approximation
0: **Form the Hilbert matrix** H:
0: **for** $i = 0$ to n **do**
0: **for** $j = 0$ to n **do**
0: Compute inner product: $H[i][j] \leftarrow \int_{-1}^{1} P_i(x)P_j(x)dx$
0: This forms the Hilbert matrix with entries $H_{i,j} = \langle P_i, P_j \rangle$
0: **end for**
0: **end for**
0: **Construct the d vector**:
0: **for** $i = 0$ to n **do**
0: Compute projection: $d[i] \leftarrow \int_{-1}^{1} f(x)P_i(x)dx$
0: This forms the vector d with entries $d_i = \langle f(x), P_i \rangle$
0: **end for**
0: **Solve the normal equations**:
0: Solve the linear system $H \cdot \mathbf{a} = d$ for coefficients $\mathbf{a}$
0: **return** $\mathbf{a}$ =0

1.3.2 Python snippet for Legendre polynomials

```python
import numpy as np
from scipy.integrate import quad

class FunctionApproximator:
    @staticmethod
    def legendre_poly(degree, x):
        """Compute Legendre polynomial P_n(x)"""
        if degree == 0:
            return np.ones_like(x)
        elif degree == 1:
            return x
        else:
            Pn_prev = np.ones_like(x)
            Pn_curr = x
            for i in range(1, degree):
                Pn_new = ((2*i + 1)*x*Pn_curr - i*Pn_prev)/(i + 1)
                Pn_prev, Pn_curr = Pn_curr, Pn_new
            return Pn_curr

    def legendre_shifted(self, degree, x):
        """Compute shifted Legendre polynomial on arbitrary interval"""
        a, b = self.default_lower, self.default_upper
        t = (2*x - (a + b)) / (b - a)  # Map to [-1, 1]
        return FunctionApproximator.legendre_poly(degree, t)

    def compute_approximation(self, degree, poly_type="legendre"):
```

```
        """Compute approximation using Legendre polynomials"""
        lower, upper = self.default_lower, self.default_upper
        poly_func = self.legendre_shifted

        # Build coefficient matrix and right-hand side vector
        A = np.zeros((degree+1, degree+1))
        Y = np.zeros(degree+1)

        for i in range(degree+1):
            for j in range(degree+1):
                integrand = lambda x: poly_func(i, x)*poly_func(j, x)
                A[i,j], _ = quad(integrand, lower, upper)
            integrand = lambda x: self.func(x)*poly_func(i, x)
            Y[i], _ = quad(integrand, lower, upper)

        # Solve the linear system
        a = np.linalg.solve(A, Y)
        return a

# Example usage:
def test_function(x):
    return (1/np.sqrt(2*np.pi))*np.exp((-x**2)/2)

approx = FunctionApproximator(test_function)
coefficients = approx.compute_approximation(3)  # Get 3rd degree approximation
print("Approximation coefficients:", coefficients)
```

1.3.3 Results

The Hilbert matrix H for degree 6 using Legendre polynomials is formed as follows:

$$H = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.67 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.40 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.29 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.22 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.18 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.15 \end{bmatrix}$$

The vector d is constructed as:

$$d^T = \begin{bmatrix} 0.68 & 0 & -0.04 & 0 & 0.00 & 0 & 0.00 \end{bmatrix}$$

The resulting coefficients are:

$$\mathbf{a}^T = \begin{bmatrix} 0.34 & 0 & -0.11 & 0 & 0.01 & 0 & 0.00 \end{bmatrix}$$

Using the resulting coefficients, the approximated polynomial is:

$$p(x) = 0.34P_0(x) - 0.11P_2(x) + 0.01P_4(x) \tag{13}$$

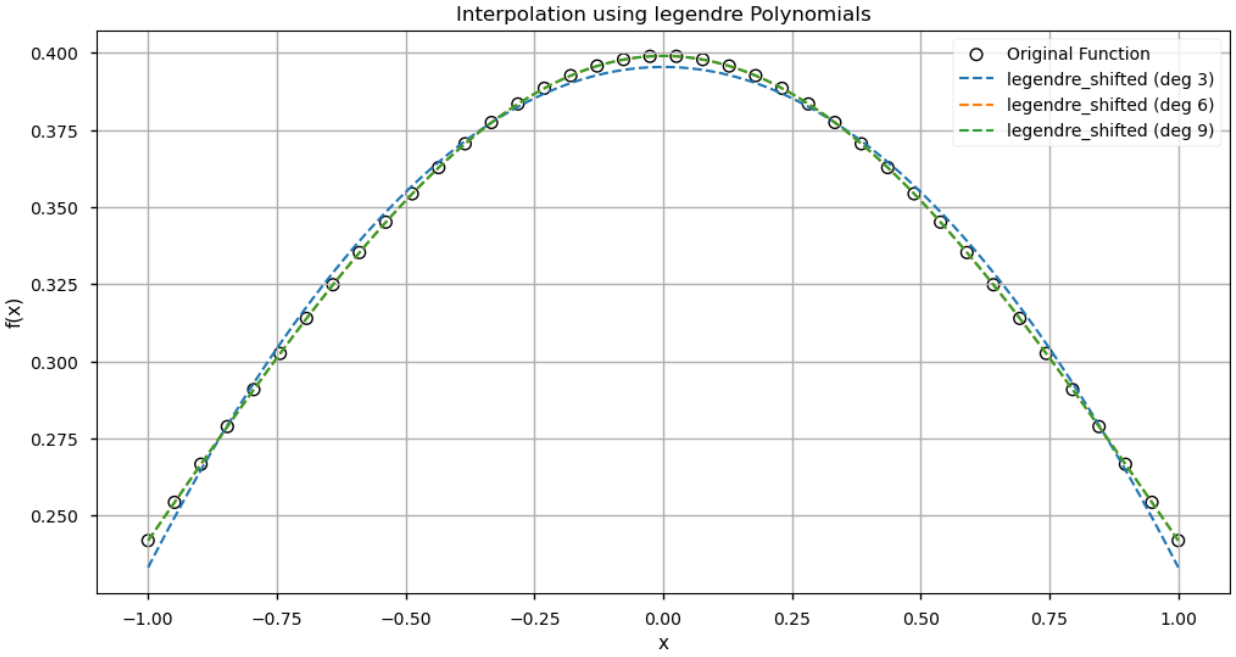


Figure 3: Interpolation method using legendre polynomials

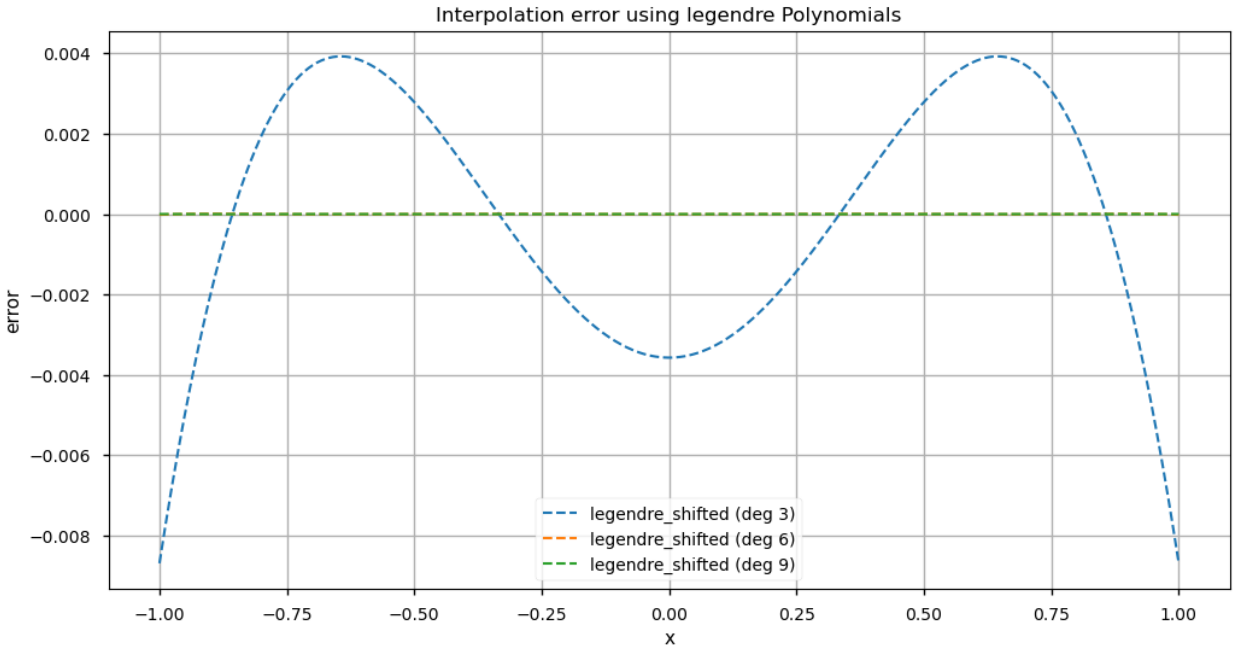


Figure 4: Interpolation error from legendre polynomials

1.3.4 Key Observations

- The Hilbert matrix H is diagonally dominant due to the orthogonality of Legendre polynomials.
- The vector d and the resulting coefficients $\mathbf{a}$ have non-zero values at even indices, which aligns with the structure of H.
- The orthogonality of Legendre polynomials simplifies the computation of the Hilbert matrix.

1.4 Chebyshev Polynomials Type 1

The Chebyshev Type 1 polynomials are defined as:

$$T_i(x) = \cos(i \arccos(x)) \tag{14}$$

A general polynomial of degree n using Chebyshev Type 1 polynomials is given by:

$$p_n(x) = a_0 T_0(x) + a_1 T_1(x) + a_2 T_2(x) + \cdots + a_n T_n(x) \tag{15}$$

The weight function for Chebyshev Type 1 polynomials is:

$$w(x) = \frac{1}{\sqrt{1 - x^2}} \tag{16}$$

The entries of the Hilbert matrix H for Chebyshev Type 1 polynomials are computed as inner products:

$$H_{i,j} = \int_{-1}^{1} T_i(x) T_j(x) \frac{1}{\sqrt{1-x^2}} dx \tag{17}$$

The entries of the d vector are computed as projections of $f(x)$ onto the Chebyshev Type 1 polynomials:

$$d_i = \int_{-1}^{1} f(x) T_i(x) \frac{1}{\sqrt{1-x^2}} dx \tag{18}$$

The normal equations to solve are:

$$H \cdot \mathbf{a} = d \tag{19}$$

where H is the Hilbert matrix, $\mathbf{a}$ is the vector of coefficients to find, and d is the vector of projections.

1.4.1 Algorithm

Algorithm 3 Chebyshev Type 1 Polynomial Approximation

Require: Function f, degree n, interval $[-1, 1]$
Ensure: Coefficients $\mathbf{a}$ for the Chebyshev Type 1 approximation
0: **Form the Hilbert matrix** H:
0: **for** $i = 0$ to n **do**
0: **for** $j = 0$ to n **do**
0: Compute inner product: $H[i][j] \leftarrow \int_{-1}^{1} T_i(x) T_j(x) \frac{1}{\sqrt{1-x^2}} dx$
0: This forms the Hilbert matrix with entries $H_{i,j} = \langle T_i, T_j \rangle$
0: **end for**
0: **end for**
0: **Construct the d vector**:
0: **for** $i = 0$ to n **do**
0: Compute projection: $d[i] \leftarrow \int_{-1}^{1} f(x) T_i(x) \frac{1}{\sqrt{1-x^2}} dx$
0: This forms the vector d with entries $d_i = \langle f(x), T_i \rangle$
0: **end for**
0: **Solve the normal equations**:
0: Solve the linear system $H \cdot \mathbf{a} = d$ for coefficients $\mathbf{a}$
0: **return** $\mathbf{a}$ =0

1.4.2 Python snippet for Chebyshev polynomials type 1

```
import numpy as np
from scipy.integrate import quad

class FunctionApproximator:
    @staticmethod
    def chebyshev_1_poly(degree, x):
        """Chebyshev polynomial of the first kind T_n(x)"""
        if degree == 0:
            return np.ones_like(x)
        elif degree == 1:
            return x
```

```
        else:
            T_prev = np.ones_like(x)
            T_curr = x
            for i in range(1, degree):
                T_new = 2 * x * T_curr - T_prev
                T_prev, T_curr = T_curr, T_new
            return T_curr

    def chebyshev_1_shifted(self, degree, x):
        """Shifted Chebyshev polynomial of the first kind"""
        a, b = self.default_lower, self.default_upper
        t = (2 * x - (a + b)) / (b - a)  # Map to [-1, 1]
        return self.chebyshev_1_poly(degree, t)

    @staticmethod
    def weight_function(poly_type, x):
        """Weight functions for different polynomial types"""
        if poly_type == "chebyshev_1":
            return 1 / np.sqrt(1 - x**2 + 1e-12)  # Type 1 weight

    def compute_approximation(self, degree, poly_type="chebyshev_1"):
        """Compute approximation using Chebyshev Type 1 polynomials"""
        lower, upper = self.default_lower, self.default_upper
        poly_func = self.chebyshev_1_shifted

        # Build coefficient matrix and right-hand side vector
        A = np.zeros((degree+1, degree+1))
        Y = np.zeros(degree+1)

        for i in range(degree+1):
            for j in range(degree+1):
                integrand = lambda x: (poly_func(i, x) * poly_func(j, x) *
                                       FunctionApproximator.weight_function(
                                           poly_type, x))
                A[i,j], _ = quad(integrand, lower, upper)
            integrand = lambda x: (self.func(x) * poly_func(i, x) *
                                   FunctionApproximator.weight_function(poly_type,
                                       x))
            Y[i], _ = quad(integrand, lower, upper)

        a = np.linalg.solve(A, Y)
        return a

# Example usage for Chebyshev Type 1
def test_function(x):
    return (1/np.sqrt(2*np.pi))*np.exp((-x**2)/2)

```

```
approx = FunctionApproximator(test_function)
type1_coeffs = approx.compute_approximation(5, 'chebyshev_1')
print("Chebyshev Type 1 coefficients:", type1_coeffs)
```

1.4.3 Results

For Chebyshev Type 1 polynomials, the Hilbert matrix H for degree 6 is:

$$H = \begin{bmatrix} 3.14 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.57 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.57 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.57 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.57 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.57 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.57 \end{bmatrix}$$

The vector d is constructed as:

$$d^T = \begin{bmatrix} 0.99 & 0 & -0.12 & 0 & 0.01 & 0 & 0.00 \end{bmatrix}$$

The resulting coefficients are:

$$\mathbf{a}^T = \begin{bmatrix} 0.32 & 0 & -0.08 & 0 & 0.00 & 0 & 0.00 \end{bmatrix}$$

Using the resulting coefficients, the approximated polynomial is:

$$p(x) = 0.32T_0(x) - 0.08T_2(x) \tag{20}$$

1.5 Chebyshev Polynomials Type 2

The Chebyshev Type 2 polynomials are defined as:

$$U_i(x) = \frac{\sin((i+1)\arccos(x))}{\sin(\arccos(x))} \tag{21}$$

A general polynomial of degree n using Chebyshev Type 2 polynomials is given by:

$$p_n(x) = a_0U_0(x) + a_1U_1(x) + a_2U_2(x) + \cdots + a_nU_n(x) \tag{22}$$

The weight function for Chebyshev Type 2 polynomials is:

$$w(x) = \sqrt{1-x^2} \tag{23}$$

The entries of the Hilbert matrix H for Chebyshev Type 2 polynomials are computed as inner products:

$$H_{i,j} = \int_{-1}^{1} U_i(x) U_j(x) \sqrt{1-x^2} dx \tag{24}$$

The entries of the d vector are computed as projections of $f(x)$ onto the Chebyshev Type 2 polynomials:

$$d_i = \int_{-1}^{1} f(x) U_i(x) \sqrt{1-x^2} dx \tag{25}$$

The normal equations to solve are:

$$H \cdot \mathbf{a} = d \tag{26}$$

where H is the Hilbert matrix, $\mathbf{a}$ is the vector of coefficients to find, and d is the vector of projections.

1.5.1 Algorithm

Algorithm 4 Chebyshev Type 2 Polynomial Approximation

Require: Function f, degree n, interval $[-1, 1]$
Ensure: Coefficients $\mathbf{a}$ for the Chebyshev Type 2 approximation
0: **Form the Hilbert matrix** H:
0: **for** $i = 0$ to n **do**
0: **for** $j = 0$ to n **do**
0: Compute inner product: $H[i][j] \leftarrow \int_{-1}^{1} U_i(x) U_j(x) \sqrt{1-x^2} dx$
0: This forms the Hilbert matrix with entries $H_{i,j} = \langle U_i, U_j \rangle$
0: **end for**
0: **end for**
0: **Construct the d vector**:
0: **for** $i = 0$ to n **do**
0: Compute projection: $d[i] \leftarrow \int_{-1}^{1} f(x) U_i(x) \sqrt{1-x^2} dx$
0: This forms the vector d with entries $d_i = \langle f(x), U_i \rangle$
0: **end for**
0: **Solve the normal equations**:
0: Solve the linear system $H \cdot \mathbf{a} = d$ for coefficients $\mathbf{a}$
0: **return a** =0

1.5.2 Python snippet for Chebyshev polynomials type 2

```
112 import numpy as np
113 from scipy.integrate import quad
114
115 class FunctionApproximator:
116     @staticmethod
117     def chebyshev_2_poly(degree, x):
118         """Chebyshev polynomial of the second kind U_n(x)"""
119         if degree == 0:
120             return np.ones_like(x)
121         elif degree == 1:
122             return 2 * x
```

```
        else:
            U_prev = np.ones_like(x)
            U_curr = 2 * x
            for i in range(1, degree):
                U_new = 2 * x * U_curr - U_prev
                U_prev, U_curr = U_curr, U_new
            return U_curr

    def chebyshev_2_shifted(self, degree, x):
        """Shifted Chebyshev polynomial of the second kind"""
        a, b = self.default_lower, self.default_upper
        t = (2 * x - (a + b)) / (b - a)  # Map to [-1, 1]
        return self.chebyshev_2_poly(degree, t)

    @staticmethod
    def weight_function(poly_type, x):
        """Weight functions for different polynomial types"""
        if poly_type == "chebyshev_2":
            return np.sqrt(1 - x**2 + 1e-12)  # Type 2 weight

    def compute_approximation(self, degree, poly_type="chebyshev_2"):
        """Compute approximation using Chebyshev Type 2 polynomials"""
        lower, upper = self.default_lower, self.default_upper
        poly_func = self.chebyshev_2_shifted

        # Build coefficient matrix and right-hand side vector
        A = np.zeros((degree+1, degree+1))
        Y = np.zeros(degree+1)

        for i in range(degree+1):
            for j in range(degree+1):
                integrand = lambda x: (poly_func(i, x) * poly_func(j, x) *
                                       FunctionApproximator.weight_function(
                                           poly_type, x))
                A[i,j], _ = quad(integrand, lower, upper)
            integrand = lambda x: (self.func(x) * poly_func(i, x) *
                                   FunctionApproximator.weight_function(poly_type,
                                       x))
            Y[i], _ = quad(integrand, lower, upper)

        a = np.linalg.solve(A, Y)
        return a

# Example usage for Chebyshev Type 2
def test_function(x):
    return (1/np.sqrt(2*np.pi))*np.exp((-x**2)/2)

```

```
approx = FunctionApproximator(test_function)
type2_coeffs = approx.compute_approximation(5, 'chebyshev_2')
print("Chebyshev Type 2 coefficients:", type2_coeffs)
```

1.5.3 Results

For Chebyshev Type 2 polynomials, the Hilbert matrix H for degree 6 is:

$$H = \begin{bmatrix} 1.57 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.57 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.57 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.57 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.57 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.57 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.57 \end{bmatrix}$$

The vector d is constructed as:

$$d^T = \begin{bmatrix} 0.56 & 0 & -0.07 & 0 & 0.00 & 0 & 0.00 \end{bmatrix}$$

The resulting coefficients are:

$$\mathbf{a}^T = \begin{bmatrix} 0.35 & 0 & -0.04 & 0 & 0.00 & 0 & 0.00 \end{bmatrix}$$

Using the resulting coefficients, the approximated polynomial is:

$$p(x) = 0.35U_0(x) - 0.04U_2(x) \tag{27}$$

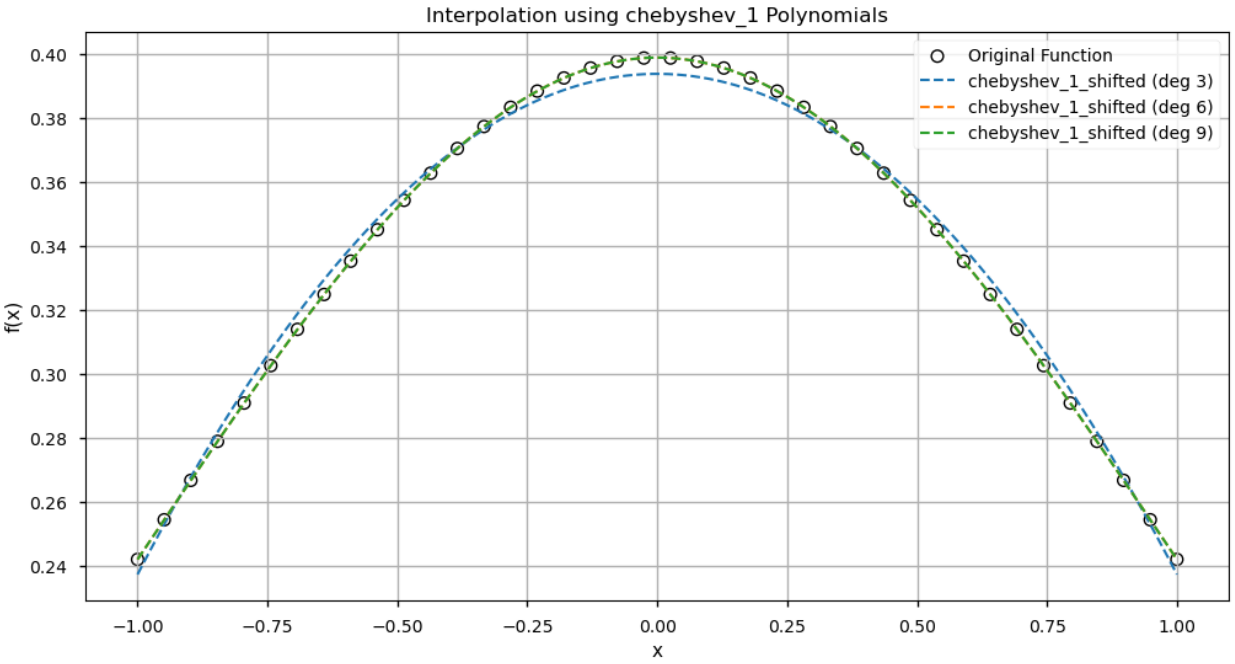


Figure 5: Interpolation method using chebyshev polynomials type 1

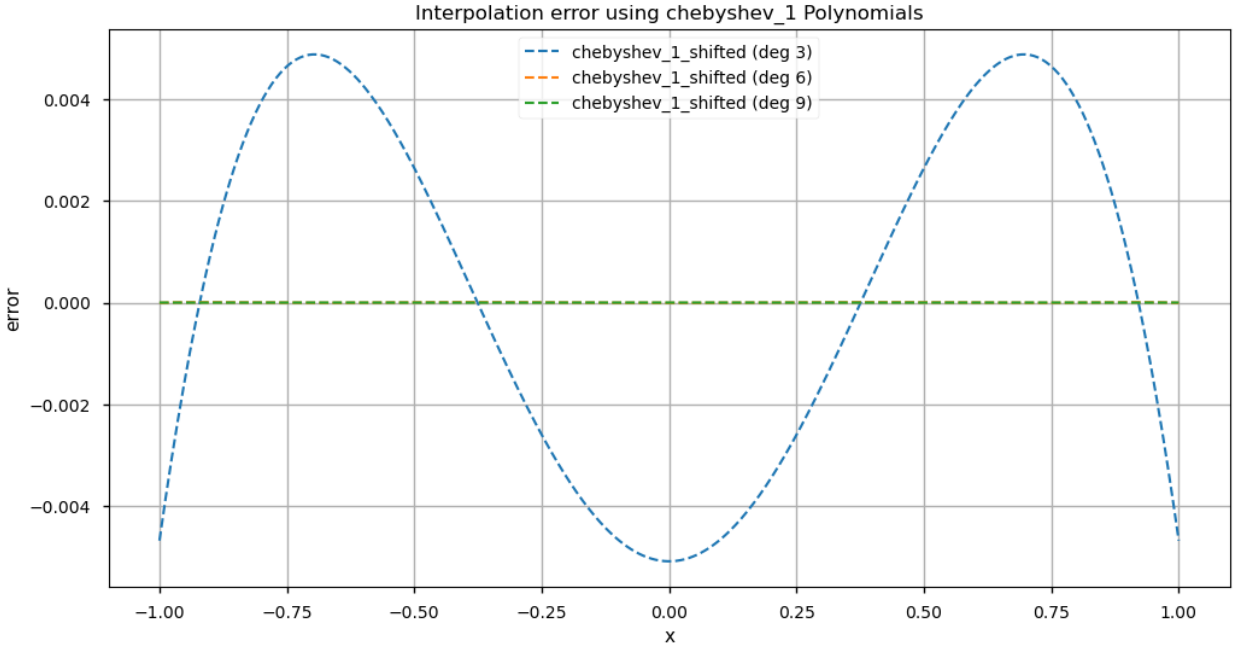


Figure 6: Interpolation error from chebyshev polynomials type 1

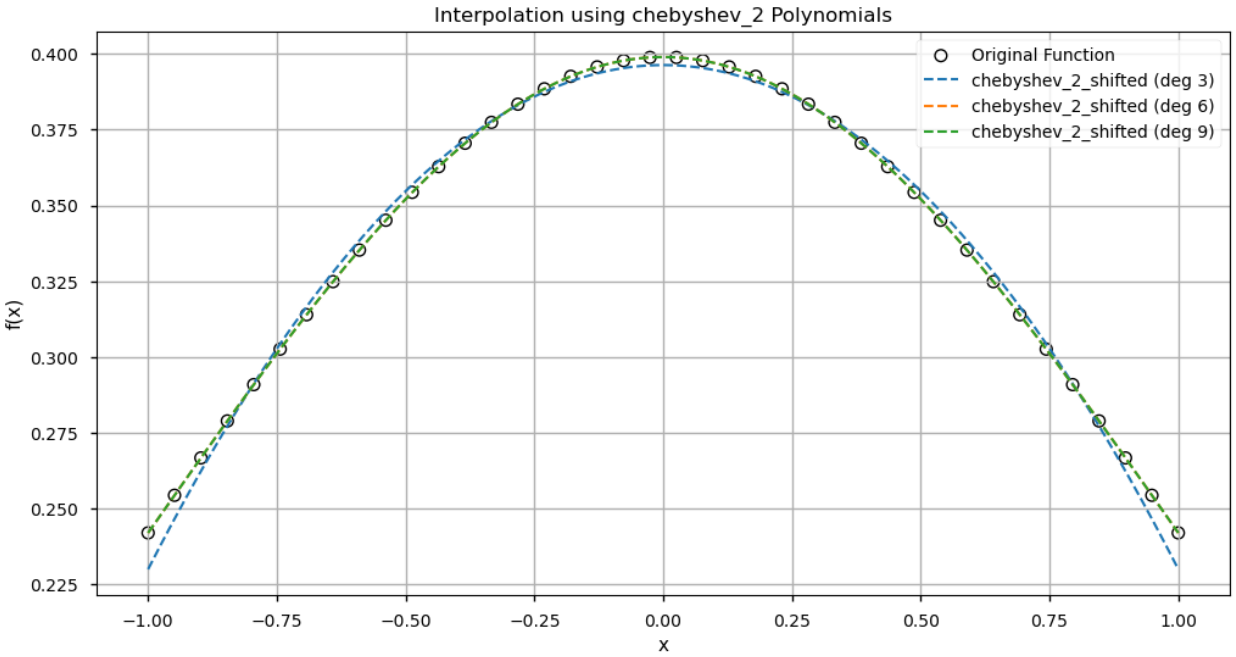


Figure 7: Interpolation method using chebyshev polynomials type 2

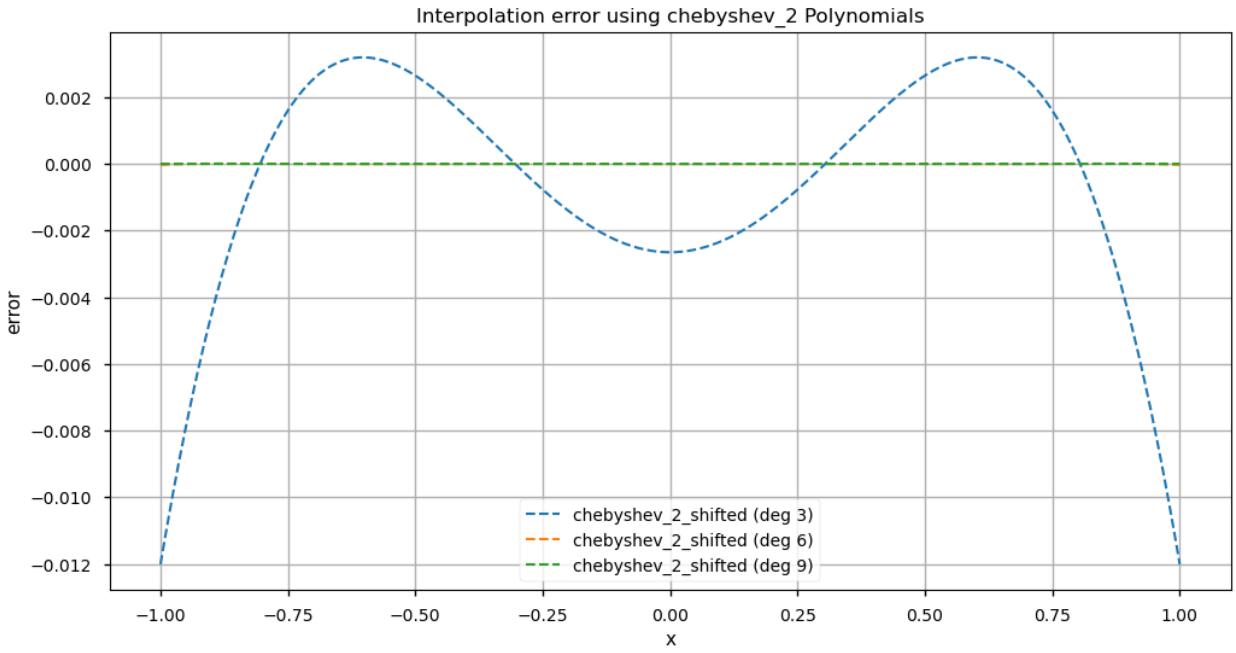


Figure 8: Interpolation error from chebyshev polynomials type 2

1.5.4 Key Observations

- The Hilbert matrices for both Chebyshev Type 1 and Type 2 polynomials are diagonally dominant.
- The vectors d and the resulting coefficients $\mathbf{a}$ have non-zero values at even indices for both types of

polynomials.

- The orthogonality of Chebyshev polynomials simplifies the computation of the Hilbert matrix.

1.6 Laguerre Polynomials

The Laguerre polynomials are defined as:

$$L_i(x) = \frac{e^x}{i!} \frac{d^i}{dx^i} \left(e^{-x} x^i \right) \tag{28}$$

A general polynomial of degree n using Laguerre polynomials is given by:

$$p_n(x) = a_0 L_0(x) + a_1 L_1(x) + a_2 L_2(x) + \cdots + a_n L_n(x) \tag{29}$$

The weight function for Laguerre polynomials is:

$$w(x) = e^{-x} \tag{30}$$

The entries of the Hilbert matrix H for Laguerre polynomials are computed as inner products:

$$H_{i,j} = \int_0^\infty L_i(x) L_j(x) e^{-x} dx \tag{31}$$

The entries of the d vector are computed as projections of $f(x)$ onto the Laguerre polynomials:

$$d_i = \int_0^\infty f(x) L_i(x) e^{-x} dx \tag{32}$$

The normal equations to solve are:

$$H \cdot \mathbf{a} = d \tag{33}$$

where H is the Hilbert matrix, $\mathbf{a}$ is the vector of coefficients to find, and d is the vector of projections.

1.6.1 Algorithm

Algorithm 5 Laguerre Polynomial Approximation

Require: Function f, degree n, interval $[0, \infty)$
Ensure: Coefficients $\mathbf{a}$ for the Laguerre approximation
Form the Hilbert matrix H:
for $i = 0$ to n **do**
  for $j = 0$ to n **do**
    Compute inner product: $H[i][j] \leftarrow \int_0^\infty L_i(x) L_j(x) e^{-x} dx$
    This forms the Hilbert matrix with entries $H_{i,j} = \langle L_i, L_j \rangle$
  end for
end for
Construct the d vector:
for $i = 0$ to n **do**
  Compute projection: $d[i] \leftarrow \int_0^\infty f(x) L_i(x) e^{-x} dx$
  This forms the vector d with entries $d_i = \langle f(x), L_i \rangle$
end for
Solve the normal equations:
Solve the linear system $H \cdot \mathbf{a} = d$ for coefficients $\mathbf{a}$
return a =0

1.6.2 Python snippet for Laguerre polynomials

```python
import numpy as np
from scipy.integrate import quad

class FunctionApproximator:
    @staticmethod
    def laguerre_poly(degree, x):
        """Laguerre polynomial L_n(x)"""
        if degree == 0:
            return np.ones_like(x)
        elif degree == 1:
            return 1 - x
        else:
            L_prev = np.ones_like(x)
            L_curr = 1 - x
            for i in range(1, degree):
                L_new = ((2 * i + 1 - x) * L_curr - i * L_prev) / (i + 1)
                L_prev, L_curr = L_curr, L_new
            return L_curr

    @staticmethod
    def weight_function(poly_type, x):
        """Weight function for Laguerre polynomials"""
        if poly_type == "laguerre":
            return np.exp(-x)  # Laguerre weight function

    def compute_approximation(self, degree, poly_type="laguerre"):
```

```
        """Compute approximation using Laguerre polynomials"""
        lower, upper = 0, np.inf  # Laguerre polynomials are defined on [0, inf)

        # Build coefficient matrix and right-hand side vector
        A = np.zeros((degree+1, degree+1))
        Y = np.zeros(degree+1)

        for i in range(degree+1):
            for j in range(degree+1):
                integrand = lambda x: (FunctionApproximator.laguerre_poly(i, x) *
                                       FunctionApproximator.laguerre_poly(j, x) *
                                       FunctionApproximator.weight_function(
                                           poly_type, x))
                A[i,j], _ = quad(integrand, lower, upper)
            integrand = lambda x: (self.func(x) *
                                   FunctionApproximator.laguerre_poly(i, x) *
                                   FunctionApproximator.weight_function(poly_type,
                                       x))
            Y[i], _ = quad(integrand, lower, upper)

        a = np.linalg.solve(A, Y)
        return a

# Example usage for Laguerre polynomials
def test_function(x):
    return (1/np.sqrt(2*np.pi))*np.exp((-x**2)/2)

approx = FunctionApproximator(test_function)
laguerre_coeffs = approx.compute_approximation(5, 'laguerre')
print("Laguerre coefficients:", laguerre_coeffs)
```

1.6.3 Results

For Laguerre polynomials, the Hilbert matrix H for degree 6 is:

$$H = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

The vector d is constructed as:

$$d^T = \begin{bmatrix} 0.26 & 0.12 & 0.05 & 0.01 & -0.01 & -0.01 & -0.01 \end{bmatrix}$$

The resulting coefficients are:

$$\mathbf{a}^T = \begin{bmatrix} 0.26 & 0.12 & 0.05 & 0.01 & -0.01 & -0.01 & -0.01 \end{bmatrix}$$

Using the resulting coefficients, the approximated polynomial is:

$$p(x) = 0.26L_0(x) + 0.12L_1(x) + 0.05L_2(x) + 0.01L_3(x) - 0.01L_4(x) - 0.01L_5(x) - 0.01L_6(x) \tag{34}$$

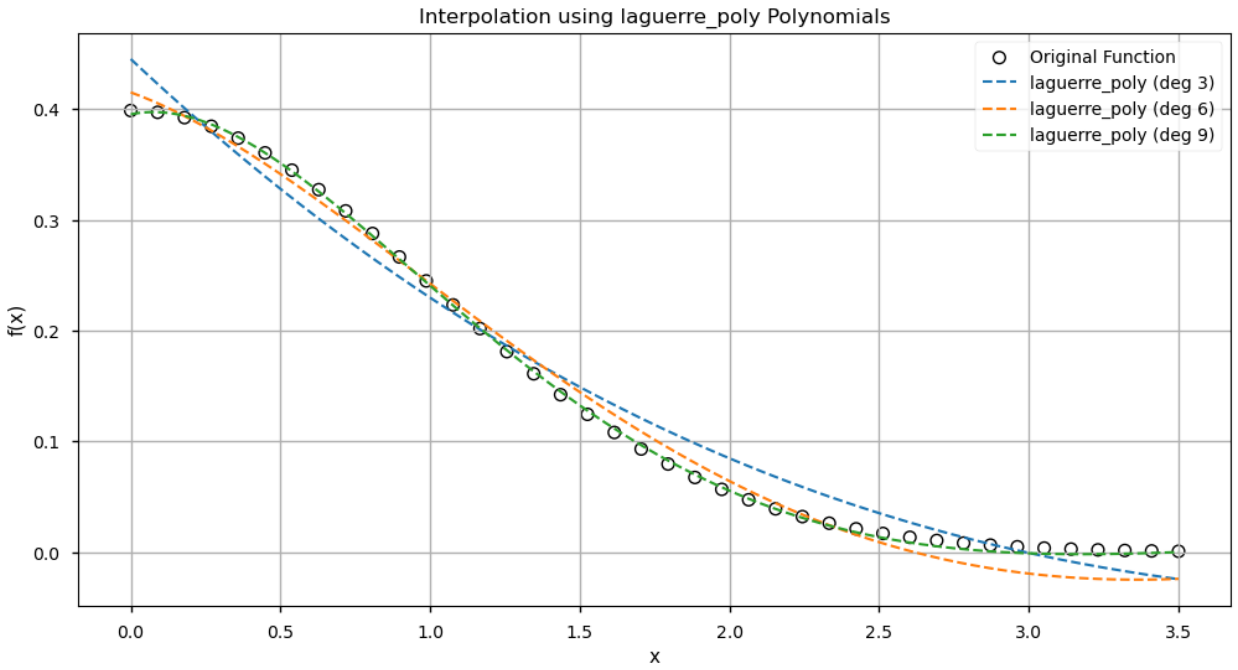


Figure 9: Interpolation method using laguerre polynomials

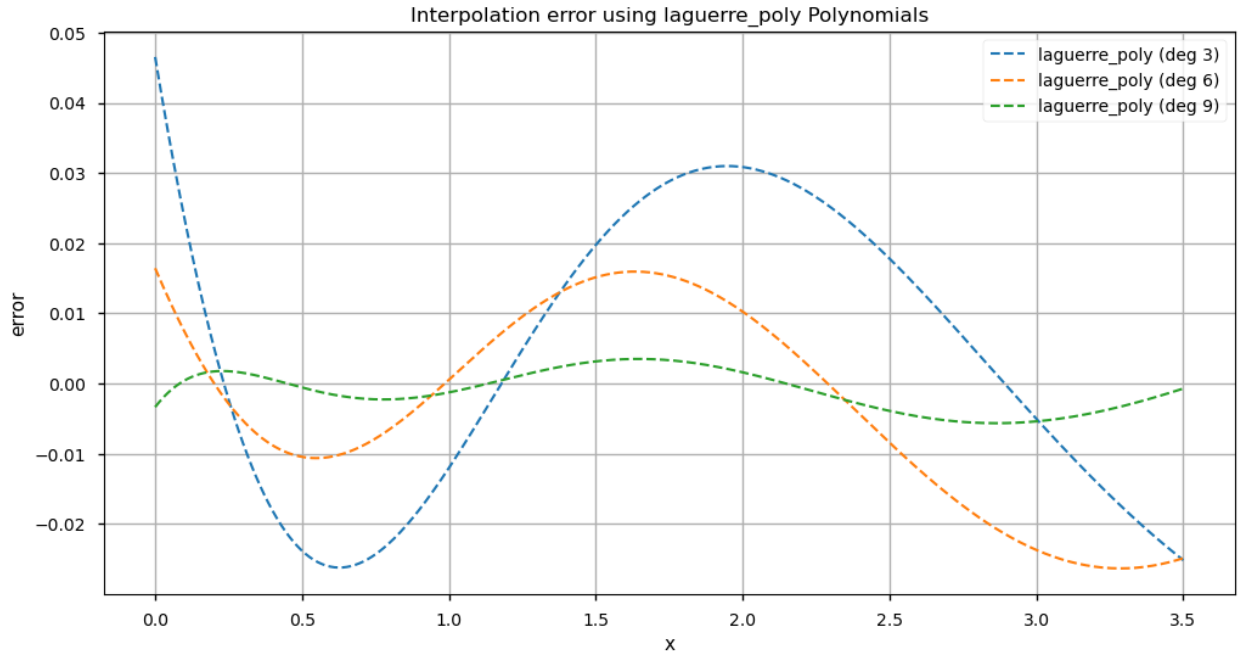


Figure 10: Interpolation error from laguerre polynomials

1.6.4 Key Observations

- The Hilbert matrix H is diagonal due to the orthogonality of Laguerre polynomials.
- The resulting coefficients $\mathbf{a}$ match the structure of H and d.
- The orthogonality of Laguerre polynomials simplifies the computation of the Hilbert matrix.

1.7 Hermite Polynomials

The Hermite polynomials are defined as:

$$H_i(x) = (-1)^i e^{x^2} \frac{d^i}{dx^i} \left(e^{-x^2} \right) \tag{35}$$

A general polynomial of degree n using Hermite polynomials is given by:

$$p_n(x) = a_0 H_0(x) + a_1 H_1(x) + a_2 H_2(x) + \cdots + a_n H_n(x) \tag{36}$$

The weight function for Hermite polynomials is:

$$w(x) = e^{-x^2} \tag{37}$$

The entries of the Hilbert matrix H for Hermite polynomials are computed as inner products:

$$H_{i,j} = \int_{-\infty}^{\infty} H_i(x) H_j(x) e^{-x^2} dx \tag{38}$$

The entries of the d vector are computed as projections of $f(x)$ onto the Hermite polynomials:

$$d_i = \int_{-\infty}^{\infty} f(x) H_i(x) e^{-x^2} dx \tag{39}$$

The normal equations to solve are:

$$H \cdot \mathbf{a} = d \tag{40}$$

where H is the Hilbert matrix, $\mathbf{a}$ is the vector of coefficients to find, and d is the vector of projections.

1.7.1 Algorithm

Algorithm 6 Hermite Polynomial Approximation

Require: Function f, degree n, interval $(-\infty, \infty)$
Ensure: Coefficients $\mathbf{a}$ for the Hermite approximation
0: **Form the Hilbert matrix** H:
0: **for** $i = 0$ to n **do**
0: **for** $j = 0$ to n **do**
0: Compute inner product: $H[i][j] \leftarrow \int_{-\infty}^{\infty} H_i(x) H_j(x) e^{-x^2} dx$
0: This forms the Hilbert matrix with entries $H_{i,j} = \langle H_i, H_j \rangle$
0: **end for**
0: **end for**
0: **Construct the d vector**:
0: **for** $i = 0$ to n **do**
0: Compute projection: $d[i] \leftarrow \int_{-\infty}^{\infty} f(x) H_i(x) e^{-x^2} dx$
0: This forms the vector d with entries $d_i = \langle f(x), H_i \rangle$
0: **end for**
0: **Solve the normal equations**:
0: Solve the linear system $H \cdot \mathbf{a} = d$ for coefficients $\mathbf{a}$
0: **return a** =0

1.7.2 Results

For Hermite polynomials, the Hilbert matrix H for degree 6 is:

$$H = \begin{bmatrix} 1.77 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3.54 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 14.18 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 85.08 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 680.62 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6806.22 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 81674.67 \end{bmatrix}$$

The vector d is constructed as:

$$d^T = \begin{bmatrix} 0.58 & 0 & -0.38 & 0 & 0.77 & 0 & -2.57 \end{bmatrix}$$

The resulting coefficients are:

$$\mathbf{a}^T = \begin{bmatrix} 0.33 & 0 & -0.03 & 0 & 0.00 & 0 & 0.00 \end{bmatrix}$$

Using the resulting coefficients, the approximated polynomial is:

$$p(x) = 0.33H_0(x) - 0.03H_2(x) \tag{41}$$

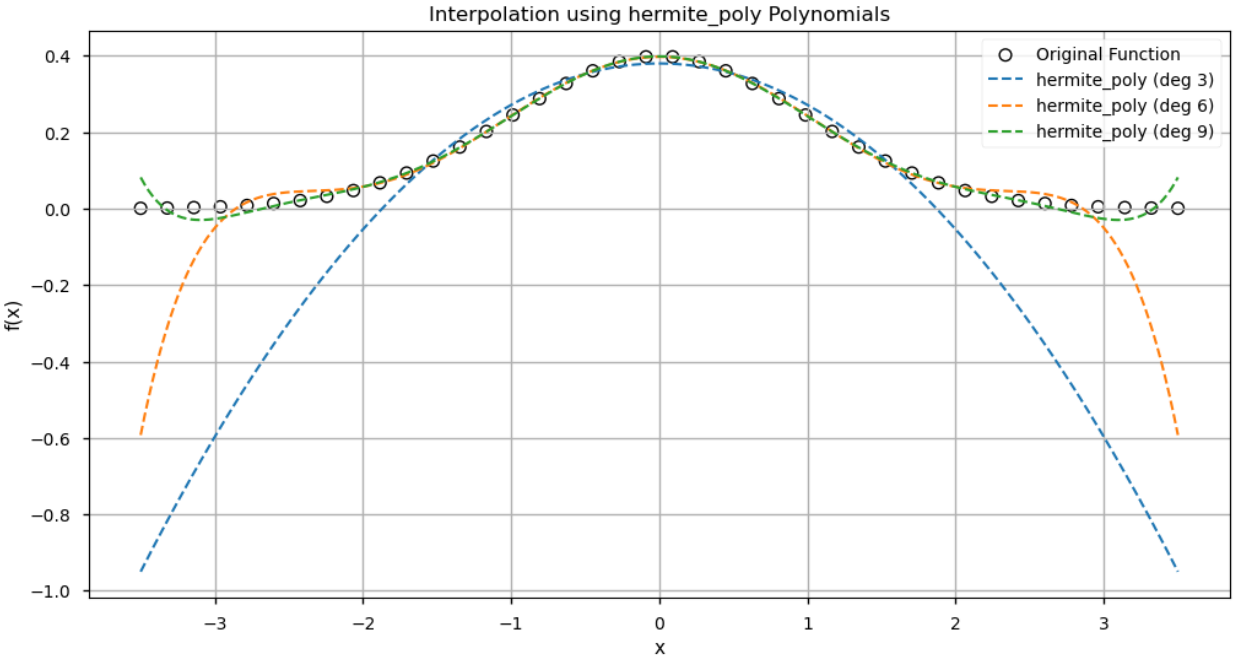


Figure 11: Interpolation method using hermite polynomials

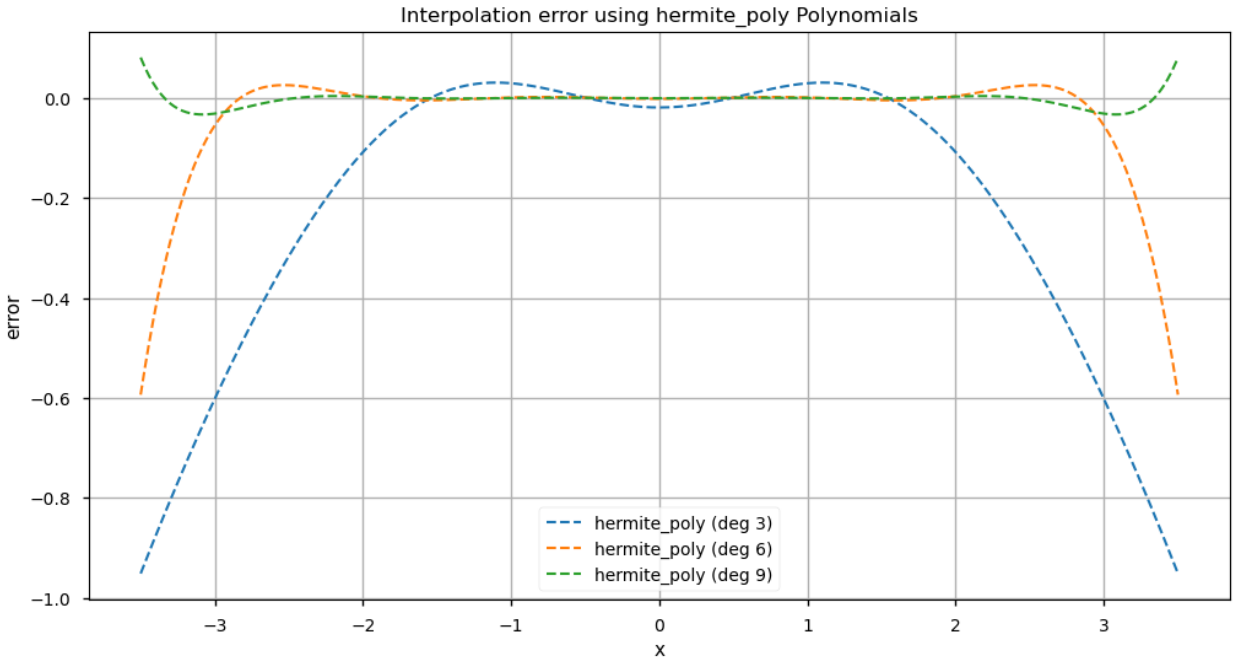


Figure 12: Interpolation error from hermite polynomials

1.7.3 Python snippet for Hermite polynomials

```python
import numpy as np
from scipy.integrate import quad

class FunctionApproximator:
    @staticmethod
    def hermite_poly(degree, x):
        """Hermite polynomial H_n(x)"""
        if degree == 0:
            return np.ones_like(x)
        elif degree == 1:
            return 2 * x
        else:
            H_prev = np.ones_like(x)
            H_curr = 2 * x
            for i in range(1, degree):
                H_new = 2 * x * H_curr - 2 * i * H_prev
                H_prev, H_curr = H_curr, H_new
            return H_curr

    @staticmethod
    def weight_function(poly_type, x):
        """Weight function for Hermite polynomials"""
        if poly_type == "hermite":
            return np.exp(-x**2)  # Hermite weight function
```

```
249
250     def compute_approximation(self, degree, poly_type="hermite"):
251         """Compute approximation using Hermite polynomials"""
252         lower, upper = -np.inf, np.inf  # Hermite polynomials are defined on (-inf
                , inf)
253
254         # Build coefficient matrix and right-hand side vector
255         A = np.zeros((degree+1, degree+1))
256         Y = np.zeros(degree+1)
257
258         for i in range(degree+1):
259             for j in range(degree+1):
260                 integrand = lambda x: (FunctionApproximator.hermite_poly(i, x) *
261                                        FunctionApproximator.hermite_poly(j, x) *
262                                        FunctionApproximator.weight_function(
                                            poly_type, x))
263                 A[i,j], _ = quad(integrand, lower, upper)
264             integrand = lambda x: (self.func(x) *
265                                    FunctionApproximator.hermite_poly(i, x) *
266                                    FunctionApproximator.weight_function(poly_type,
                                        x))
267             Y[i], _ = quad(integrand, lower, upper)
268
269         a = np.linalg.solve(A, Y)
270         return a
271
272 # Example usage for Hermite polynomials
273 def test_function(x):
274     return (1/np.sqrt(2*np.pi))*np.exp((-x**2)/2)
275
276 approx = FunctionApproximator(test_function)
277 hermite_coeffs = approx.compute_approximation(5, 'hermite')
278 print("Hermite coefficients:", hermite_coeffs)
```

1.7.4 Key Observations

- The Hilbert matrix H is diagonally dominant due to the orthogonality of Hermite polynomials.
- The resulting coefficients $\mathbf{a}$ have non-zero values at even indices, which aligns with the structure of H and d.
- The orthogonality of Hermite polynomials simplifies the computation of the Hilbert matrix.

2 Least Square

2.1 Real Case: Mechanical Properties of Steel

This study explores the relationship between steel composition, temperature conditions, and mechanical properties using least squares polynomial approximation. The dataset contains tension test results for various steel alloys tested under different temperatures. Our goal is to quantify how chemical elements and temperature influence critical mechanical properties: yield strength (YS), ultimate tensile strength (UTS), elongation (EL), and reduction of area (RA).

Table 1: Sample Data from merged_data.csv (Part 1)

Sample	C (wt%)	Si (wt%)	Mn (wt%)	P (wt%)	S (wt%)	Ni (wt%)	Cr (wt%)	Mo (wt%)
1	0.12	0.34	1.23	0.021	0.015	0.01	0.02	0.01
2	0.20	0.45	1.45	0.023	0.018	0.01	0.02	0.01
3	0.18	0.30	1.35	0.020	0.012	0.01	0.02	0.01
4	0.25	0.50	1.50	0.025	0.020	0.01	0.02	0.01
5	0.15	0.35	1.30	0.018	0.010	0.01	0.02	0.01
6	0.22	0.40	1.40	0.022	0.016	0.01	0.02	0.01
7	0.19	0.38	1.42	0.021	0.014	0.01	0.02	0.01
8	0.24	0.48	1.55	0.024	0.019	0.01	0.02	0.01

Table 2: Sample Data from merged_data.csv (Part 2)

Sample	Cu (wt%)	Ti (wt%)	Al (wt%)	B (wt%)	N (wt%)	V (wt%)	Co (wt%)	Nb+Ta (wt%)
1	0.01	0.01	0.02	0.0025	0.005	0.01	0.01	0.01
2	0.01	0.01	0.03	0.0030	0.006	0.01	0.01	0.01
3	0.01	0.01	0.02	0.0020	0.004	0.01	0.01	0.01
4	0.01	0.01	0.03	0.0035	0.007	0.01	0.01	0.01
5	0.01	0.01	0.02	0.0022	0.004	0.01	0.01	0.01
6	0.01	0.01	0.02	0.0028	0.005	0.01	0.01	0.01
7	0.01	0.01	0.02	0.0026	0.005	0.01	0.01	0.01
8	0.01	0.01	0.03	0.0032	0.006	0.01	0.01	0.01

Table 3: Sample Data from merged_data.csv (Part 3)

Sample	Temperature (K)	YS (MPa)	UTS (MPa)	EL (%)	RA (%)
1	298	450	620	25	60
2	298	520	710	20	55
3	373	410	580	30	70
4	373	550	750	22	50
5	448	380	550	35	75
6	448	500	680	28	60
7	523	350	520	40	80
8	523	480	650	25	65

Steel's mechanical properties are influenced by:

Table 4: Summary Statistics for merged_data.csv (Part 1)

Statistic	C (wt%)	Si (wt%)	Mn (wt%)	P (wt%)	S (wt%)	Ni (wt%)
Count	994	994	994	994	994	994
Mean	0.18	0.74	1.36	0.02	0.01	17.49
Std Dev	0.16	0.30	0.33	0.01	0.01	8.25
Min	0.04	0.22	0.48	0.01	0.00	8.79
25%	0.06	0.54	1.12	0.02	0.01	12.06
50%	0.07	0.62	1.47	0.02	0.01	13.21
75%	0.37	0.92	1.60	0.02	0.01	21.42
Max	0.52	1.62	1.82	0.04	0.03	35.63

Table 5: Summary Statistics for merged_data.csv (Part 2)

Statistic	Cr (wt%)	Mo (wt%)	Cu (wt%)	Ti (wt%)	Al (wt%)	B (wt%)
Count	994	938	966	938	938	700
Mean	20.82	0.39	0.17	0.12	0.05	0.00
Std Dev	3.55	0.75	0.49	0.18	0.10	0.00
Min	16.42	0	0.01	0	0	0.00
25%	17.86	0.03	0.05	0.01	0.00	0.00
50%	18.70	0.07	0.07	0.02	0.01	0.00
75%	24.90	0.25	0.12	0.06	0.04	0.00
Max	27.49	2.38	3.05	0.55	0.52	0.00

Table 6: Summary Statistics for merged_data.csv (Part 3)

Statistic	N (wt%)	V (wt%)	Co (wt%)	Nb+Ta (wt%)	Fe (wt%)	Temperature (K)
Count	980	126	560	714	994	994
Mean	0.04	0.04	0.20	0.20	58.38	58.38
Std Dev	0.04	0.00	0.15	0.32	10.58	10.58
Min	0.01	0.03	0.00	0	34.31	34.31
25%	0.02	0.03	0.04	0.01	51.05	51.05
50%	0.03	0.03	0.23	0.01	64.84	64.84
75%	0.05	0.04	0.31	0.46	66.57	66.57
Max	0.27	0.04	0.54	0.88	69.69	69.69

Table 7: Summary Statistics for merged_data.csv (Part 4)

Statistic	YS (MPa)	UTS (MPa)	EL (%)	RA (%)
Count	773	773	773	773
Mean	533.93	174.87	408.23	40.35
Std Dev	286.38	47.20	122.74	17.10
Min	25	35	20	8
25%	300	148	337	29
50%	575	171	436	40
75%	750	200	488	47
Max	1000	342	711	128

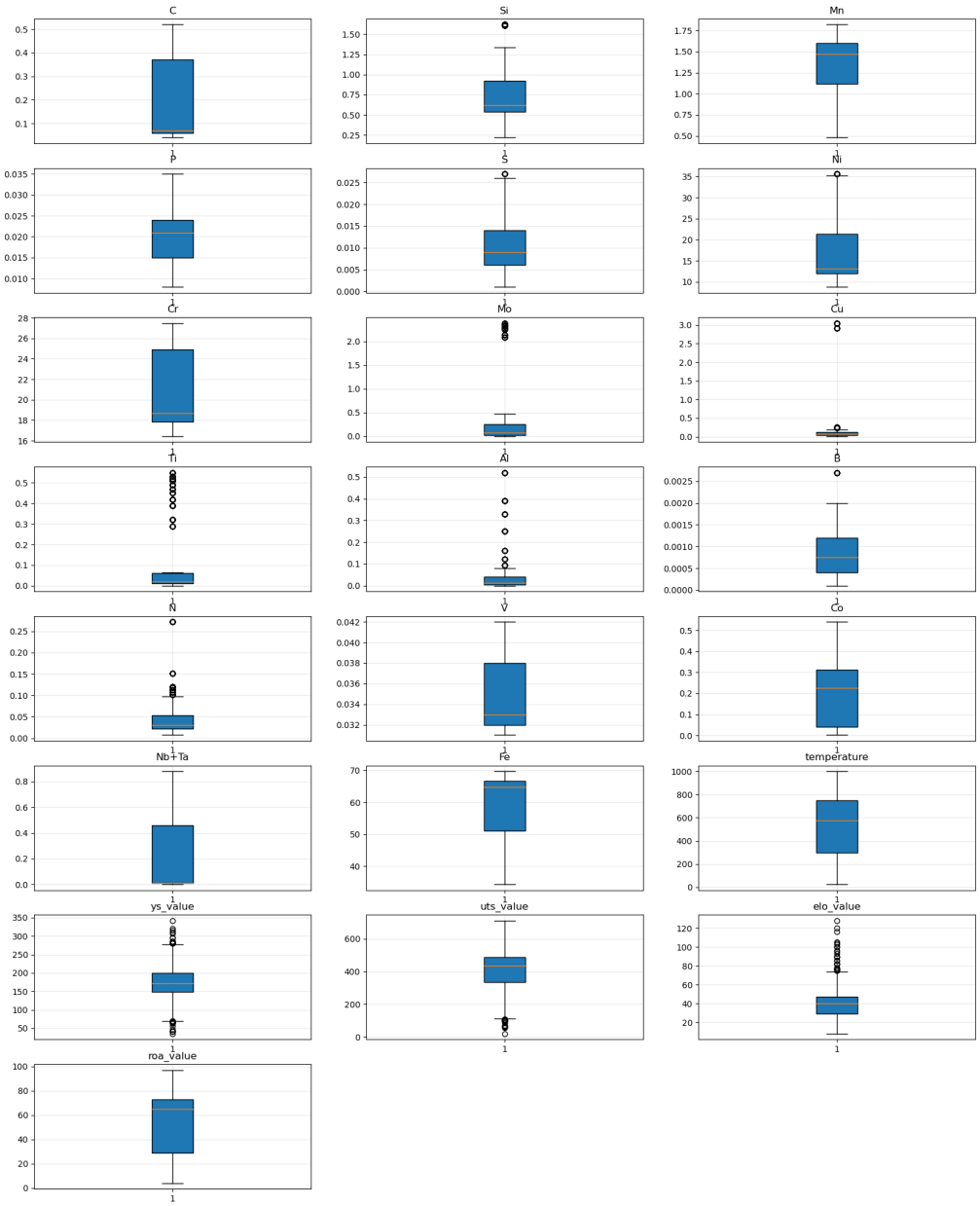


Figure 13: Descriptive statistic of merged_data.csv

- **Chemical composition**: Elements like Carbon (C), Manganese (Mn), and Boron (B) significantly affect strength and ductility
- **Temperature**: Thermal conditions during testing alter material behavior, with higher temperatures generally reducing strength and increasing ductility
- **Microstructure**: Resulting from chemical composition and thermal history

The general polynomial approximation of degree n is given by:

$$p_n(x) = \sum_{i=0}^{n} a_i x^i \tag{42}$$

For our analysis, we primarily use first-degree polynomial approximation:

$$p_1(x) = a_0 + a_1 x \tag{43}$$

This linear model provides a fundamental understanding of the relationship between independent variables (chemical elements and temperature) and dependent variables (mechanical properties).

2.2 Least Squares Method

The least squares method minimizes the sum of the squares of the residuals (differences between observed and predicted values). The goal is to find coefficients a_0 and a_1 that minimize the residual sum of squares (RSS):

$$RSS = \sum_{i=1}^{n} (y_i - (a_0 + a_1 x_i))^2 \tag{44}$$

The Gram matrix G is constructed using the inner products of the basis functions. For a first-degree polynomial, the basis functions are 1 and x. The entries of the Gram matrix are computed as:

$$G_{i,j} = \sum_{k=1}^{n} x_k^{i+j} \tag{45}$$

The normal equations for this problem are given by:

$$\begin{bmatrix} n & \sum_{i=1}^{n} x_i \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i y_i \end{bmatrix} \tag{46}$$

2.2.1 Algorithm

Algorithm 7 Least Squares Fit using General Polynomial Approximation

Require: Data points x_i, y_i, degree $n = 1$
Ensure: Coefficients $\mathbf{a} = [a_0, a_1]$
0: **Form the Gram matrix** G:
0: $G[0][0] \leftarrow n$
0: $G[0][1] \leftarrow G[1][0] \leftarrow \sum_{i=1}^{n} x_i$
0: $G[1][1] \leftarrow \sum_{i=1}^{n} x_i^2$
0: **Form the d vector**:
0: $d[0] \leftarrow \sum_{i=1}^{n} y_i$
0: $d[1] \leftarrow \sum_{i=1}^{n} x_i y_i$
0: **Solve the normal equations**:
0: Solve the linear system $G \cdot \mathbf{a} = d$ for coefficients $\mathbf{a}$
0: **return a** =0

2.2.2 Python snippet for Least Square

```python
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import os

# Load data and create directories
df = pd.read_csv('03_leastsq/merged_data.csv')
os.makedirs('03_leastsq/plots', exist_ok=True)
os.makedirs('03_leastsq/results', exist_ok=True)

# Define least squares function
def least_squares_fit(x, y, n):
    G = np.zeros((n+1, n+1))
    b = np.zeros(n+1)
    for j in range(n+1):
        for k in range(n+1):
            G[j, k] = np.sum(x**(j + k))
        b[j] = np.sum(y * x**j)
    try:
        beta = np.linalg.solve(G, b)
    except np.linalg.LinAlgError:
        beta = np.linalg.pinv(G) @ b  # Fallback to pseudo-inverse
    return beta, G, b

# Define variables and y-axis limits
y_cols = ['ys_value', 'uts_value', 'elo_value', 'roa_value']
X_cols = ['C', 'Si', 'Mn', 'P', 'S', 'Ni', 'Cr', 'Mo', 'Cu', 'Ti', 'Al', 'B', 'N',
     'V', 'Co', 'Nb+Ta', 'temperature']
ylims_dict = {
    'ys_value': (0, 400),
    'uts_value': (0, 800),
```

```
    'elo_value': (0, 120),
    'roa_value': (0, 120)
}

# Initialize results dictionary
beta_results = {}

# Process each variable combination
degrees = [1]
for x_name in X_cols:
    x = df[x_name].values
    for y_name in y_cols:
        y = df[y_name].values
        valid_mask = ~np.isnan(x) & ~np.isnan(y)
        x_valid = x[valid_mask]
        y_valid = y[valid_mask]

        if len(x_valid) == 0:
            continue

        for degree in degrees:
            beta, G, b = least_squares_fit(x_valid, y_valid, degree)
            y_pred = np.polyval(beta[::-1], x_valid)
            l2_norm = np.linalg.norm(y_valid - y_pred)

            # Save coefficients
            if y_name not in beta_results:
                beta_results[y_name] = {}
            beta_results[y_name][x_name] = {
                'beta_0': beta[0] if len(beta) > 0 else None,
                'beta_1': beta[1] if len(beta) > 1 else None
            }

            # Save results to Excel
            with pd.ExcelWriter(f"03_leastsq/results/{x_name}_vs_{y_name}_deg{
                degree}.xlsx") as writer:
                pd.DataFrame(beta, columns=['Coefficients']).to_excel(writer,
                    sheet_name='Coefficients')
                pd.DataFrame(G).to_excel(writer, sheet_name='Gram_Matrix')
                pd.DataFrame(b, columns=['RHS']).to_excel(writer, sheet_name='RHS'
                    )
                pd.DataFrame({'L2_Norm': [l2_norm]}).to_excel(writer, sheet_name='
                    Metrics', index=False)

# Generate bar charts for each dependent variable
for y_name in y_cols:
    if y_name not in beta_results:
```

```
        continue

    x_vars = []
    beta1_values = []
    for x_name in X_cols:
        if x_name in beta_results[y_name]:
            x_vars.append(x_name)
            beta1 = beta_results[y_name][x_name]['beta_1']
            beta1_values.append(beta1 if beta1 is not None else 0)

    plt.figure(figsize=(12, 6))
    plt.bar(x_vars, beta1_values, color='blue')
    plt.xlabel('Independent Variables')
    plt.ylabel('Beta_1 Coefficient')
    plt.yscale('symlog')
    plt.title(f'Beta_1 Coefficients for {y_name}')
    plt.xticks(rotation=45, ha='right')
    plt.grid(axis='y', linestyle='--', alpha=0.7)
    plt.tight_layout()
    plt.savefig(f'03_leastsq/plots/bar_charts/{y_name}_beta1_bar_chart.png')
    plt.close()

# Save beta coefficients to Excel
beta_df = pd.DataFrame(beta_results).T
beta_df.to_excel("03_leastsq/results/beta_coefficients.xlsx")

print("Beta coefficients collected and saved.")
```

2.3 Results

Our analysis reveals several important relationships:

2.3.1 Example 1: Temperature vs Yield Strength

- **Gram matrix**:

$$G = \begin{bmatrix} 773 & 364,875 \\ 364,875 & 228,744,375 \end{bmatrix}$$

- **d vector**:

$$d = \begin{bmatrix} 135,174 \\ 55,810,200 \end{bmatrix}$$

- **Coefficients**:

$$\mathbf{a} = \begin{bmatrix} 241.65 \\ -0.14 \end{bmatrix}$$

The negative coefficient for temperature indicates that yield strength decreases with increasing temperature, which aligns with expected material behavior as higher temperatures reduce material strength.

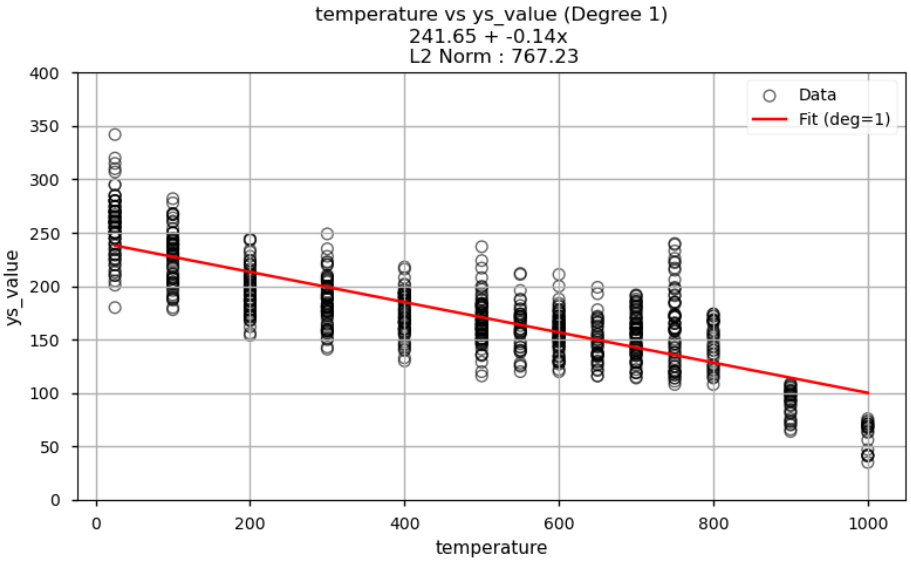


Figure 14: Relationship between temperature (in Kelvin) and Yield Strength (in MPa)

2.3.2 Example 2: Boron vs Yield Strength

- **Gram matrix**:

$$G = \begin{bmatrix} 565 & 0.48 \\ 0.48 & 0.00 \end{bmatrix}$$

- **d vector**:

$$d = \begin{bmatrix} 99,733 \\ 86.47 \end{bmatrix}$$

- **Coefficients**:

$$\mathbf{a} = \begin{bmatrix} 171.24 \\ 6,176.45 \end{bmatrix}$$

Boron shows a strong positive correlation with yield strength, demonstrating its effectiveness as a microalloying element in enhancing steel strength.

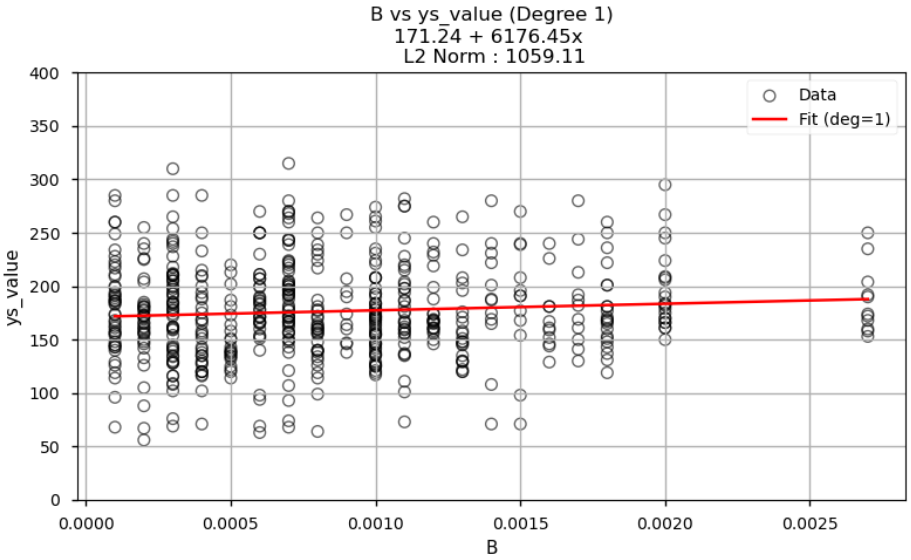


Figure 15: Relationship between Boron (wt%) and Yield Strength (in MPa)

2.3.3 Example 3: Carbon vs Reduction of Area

- **Gram matrix**:

$$G = \begin{bmatrix} 773 & 138.07 \\ 138.07 & 45.09 \end{bmatrix}$$

- **d vector**:

$$d = \begin{bmatrix} 42,137 \\ 5,132.12 \end{bmatrix}$$

- **Coefficients**:

$$\mathbf{a} = \begin{bmatrix} 75.45 \\ -117.23 \end{bmatrix}$$

Carbon content exhibits a negative relationship with reduction of area, indicating that higher carbon levels reduce ductility.

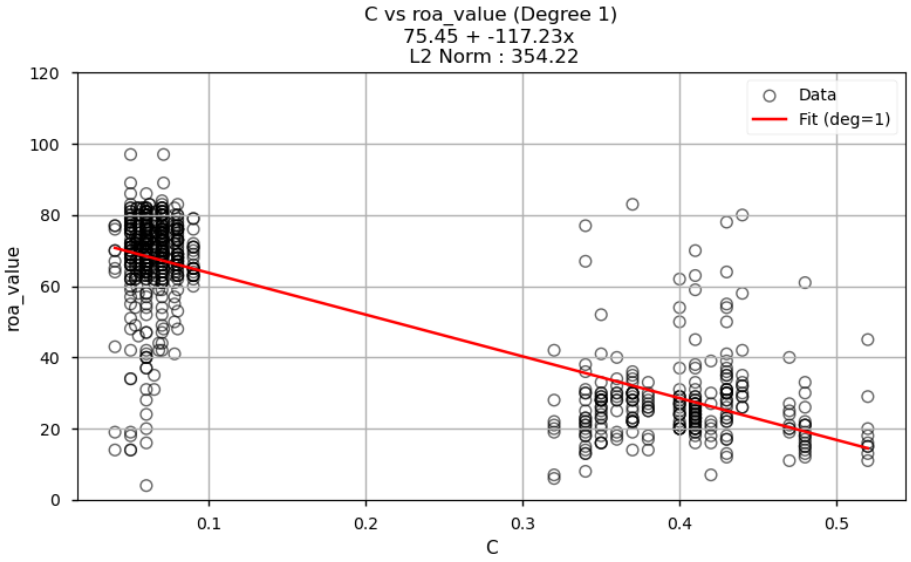


Figure 16: Relationship between Carbon (wt%) and Reduction of Area (in %)

2.3.4 Example 4: Silicon vs Elongation

- **Gram matrix**:

$$G = \begin{bmatrix} 773 & 562.02 \\ 562.02 & 473.82 \end{bmatrix}$$

- **d vector**:

$$d = \begin{bmatrix} 31,188 \\ 20,852.98 \end{bmatrix}$$

- **Coefficients**:

$$\mathbf{a} = \begin{bmatrix} 60.67 \\ -27.96 \end{bmatrix}$$

Silicon also shows a negative relationship with elongation, suggesting that increased silicon content reduces steel ductility.

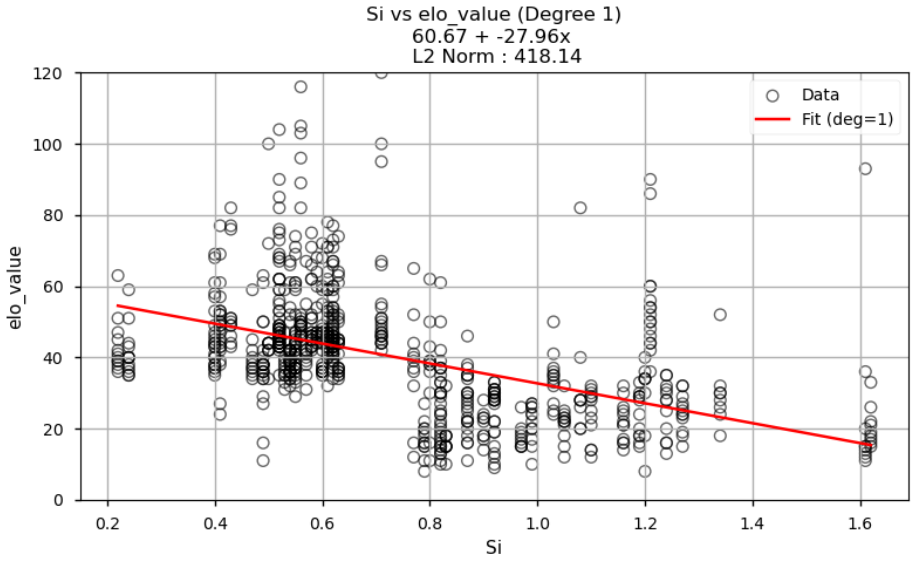


Figure 17: Relationship between Silicon (wt%) and Elongation (in %)

The following bar charts illustrate the beta coefficients for each independent variable across different mechanical properties:

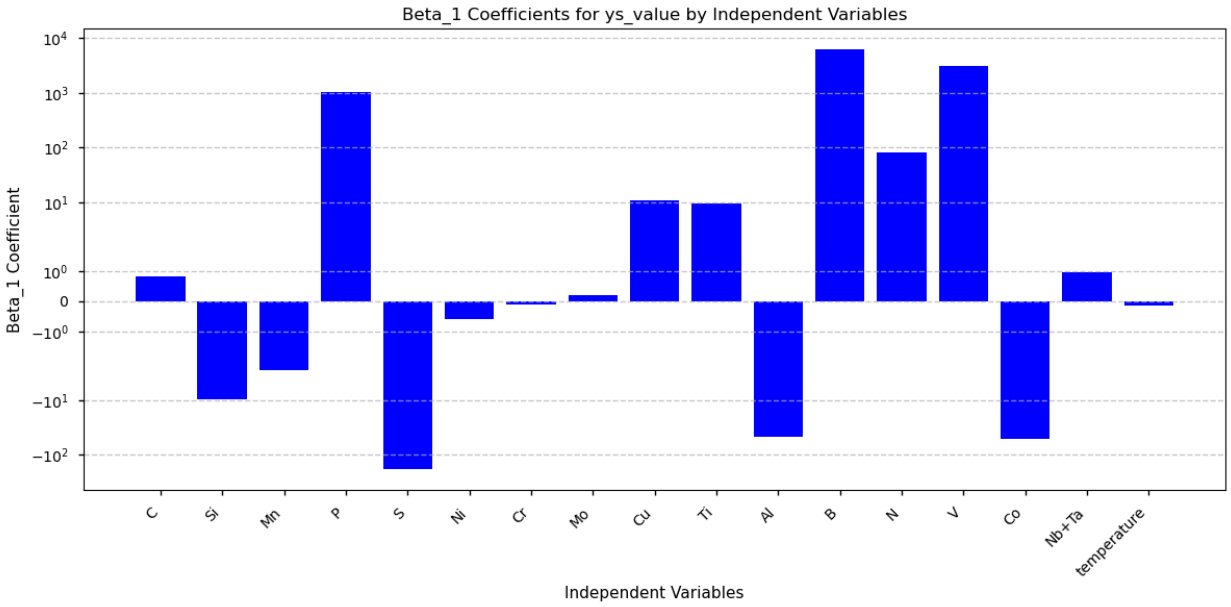


Figure 18: Relationship between independent variables and Yield Strength (in MPa)

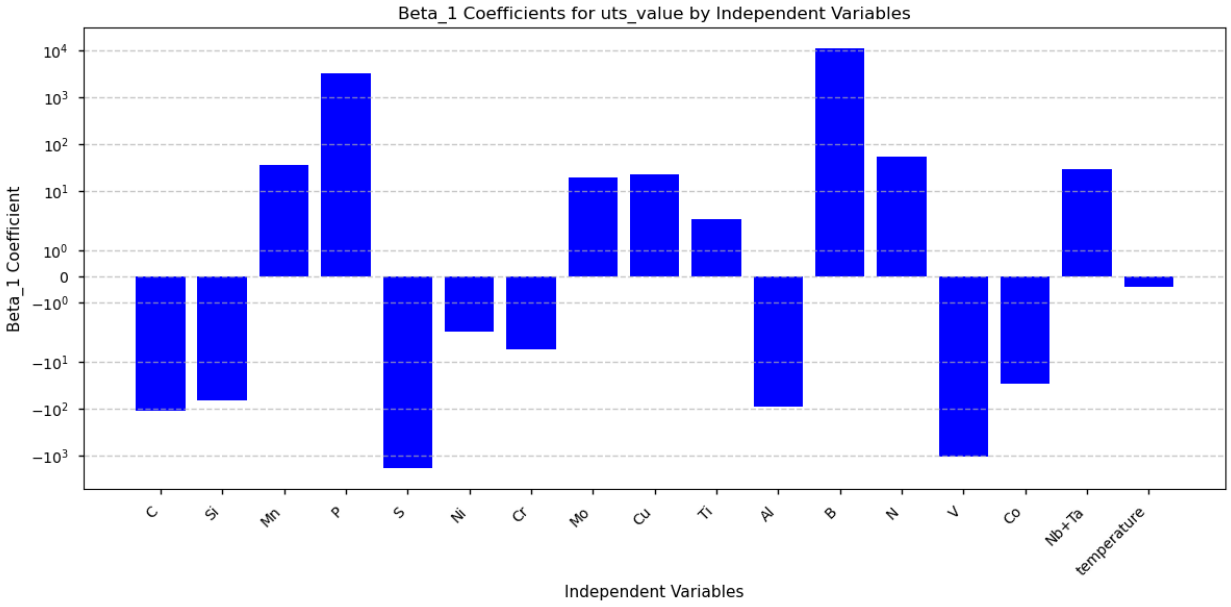


Figure 19: Relationship between independent variables and Ultimate Tensile Strength (in MPA)

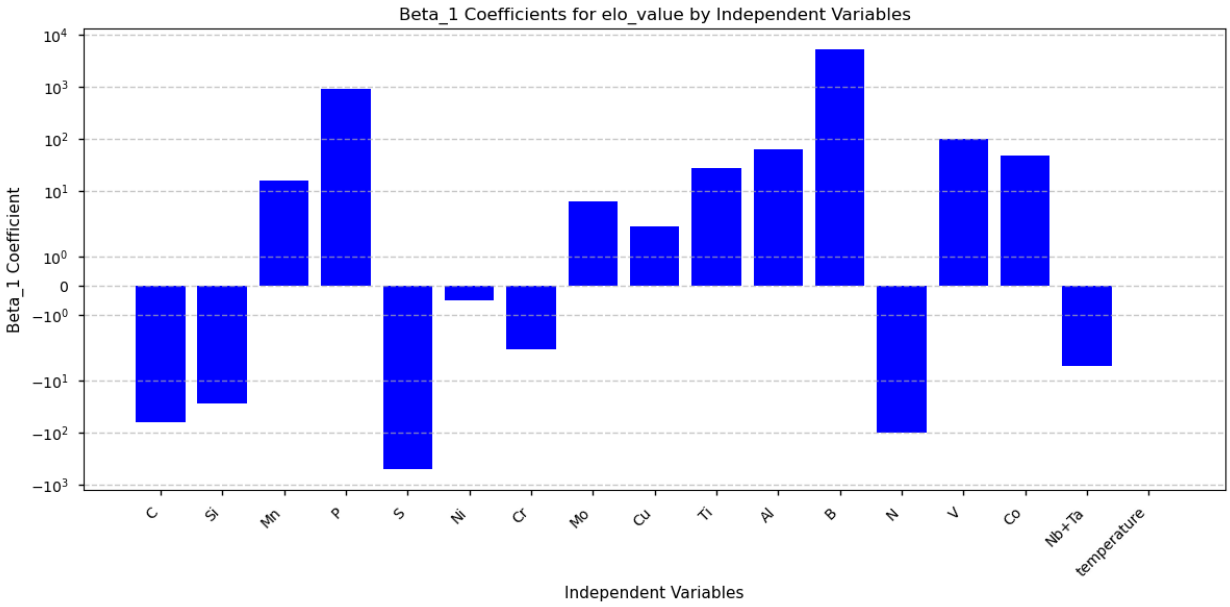


Figure 20: Relationship between independent variables and %Elongation

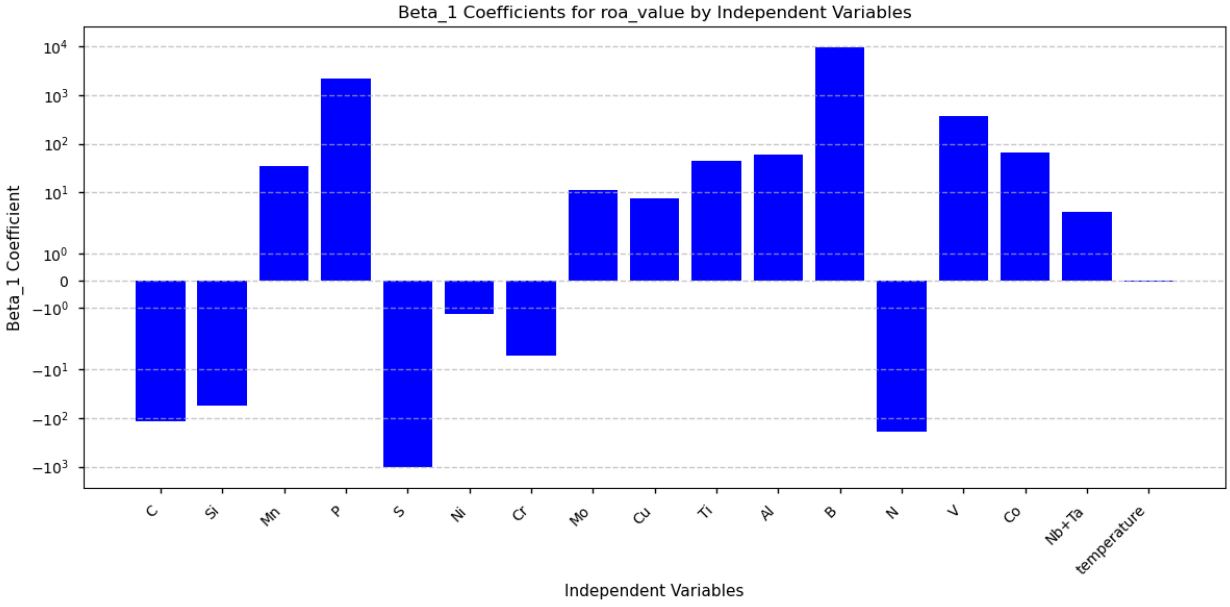


Figure 21: Relationship between independent variables and %Reduction of Area

2.4 Key Observations

- The Gram matrix G is symmetric and positive definite, ensuring a unique solution for the normal equations.
- The coefficients $\mathbf{a}$ provide the best linear approximation for the relationship between variables.
- The signs of a_1 indicate the direction of the relationship between independent variables and mechanical properties:
  - Positive coefficients: Strengthening elements (e.g., Boron for YS)
  - Negative coefficients: Ductility-reducing elements (e.g., Carbon for RA)
- Elements like Carbon and Silicon generally reduce ductility while increasing strength, demonstrating the typical strength-ductility trade-off in steels.
- Boron shows exceptional effectiveness in increasing yield strength despite its low concentration.
- **Important Note:** While we observe correlations between variables, it is crucial to remember that correlation does not imply causation. These relationships should be validated through further experimental and mechanistic studies before drawing definitive conclusions about causal relationships.

This least squares analysis provides valuable insights into how chemical composition and temperature affect steel's mechanical properties. The results can guide steel selection and alloy design by quantifying the impact of specific elements and testing conditions. Further analysis using higher-degree polynomials or multivariate models could provide more comprehensive understanding of these relationships.

3 Integration

3.1 Real Case: Calculation of Enthalpy

The calculation of sensible heat for materials like calcium oxide (CaO) involves evaluating integrals of thermodynamic functions. The enthalpy change of CaO over a temperature range can be expressed as:

$$\Delta H = \int_{T_1}^{T_2} C_p(T) dT \tag{47}$$

Where $C_p(T)$ is the temperature-dependent specific heat capacity. Due to the complexity of $C_p(T)$ functions, analytical integration is often impractical, necessitating numerical approximation methods.

For example, the heat capacity of CaO is modeled by:

$$C_p(T) = 57.753 + (-10.779) \times 10^{-3} T + (-11.51) \times 10^{5} T^{-2} + 5.328 \times 10^{-6} T^{2} \tag{48}$$

3.2 Method

3.2.1 Left Rectangular Method

This method approximates the integral using rectangles built on left endpoints. The formula is:

$$\int_a^b f(x)dx \approx h \sum_{i=0}^{n-1} f(a + i \cdot h) \tag{49}$$

Algorithm 8 Left Rectangular Integration

Require: Function f, interval $[a, b]$, number of subintervals n
Ensure: Approximation of $\int_a^b f(x)dx$
0: $h \leftarrow \frac{b-a}{n}$
0: $S \leftarrow 0$
0: **for** $i = 0$ to $n - 1$ **do**
0: $\quad S \leftarrow S + f(a + i \cdot h) \cdot h$
0: **end for**
0: **return** S =0

Python snippet for the left rectangle method:

```
379 def left_rectangular(f, a, b, n):
380     h = (b - a)/n
381     x = np.linspace(a, b, n+1)[:-1]
382     return h * np.sum(f(x))
```

This method provides a lower bound approximation for monotonically increasing functions.

3.2.2 Right Rectangular Method

The right endpoint variant calculates:

$$\int_a^b f(x)dx \approx h \sum_{i=1}^{n} f(a + i \cdot h) \tag{50}$$

Algorithm 9 Right Rectangular Integration

Require: Function f, interval $[a, b]$, number of subintervals n
Ensure: Approximation of $\int_a^b f(x)dx$
0: $h \leftarrow \frac{b-a}{n}$
0: $S \leftarrow 0$
0: **for** $i = 1$ to n **do**
0: $\quad S \leftarrow S + f(a + i \cdot h) \cdot h$
0: **end for**
0: **return** S =0

Python snippet for the right rectangle method:

```
def right_rectangular(f, a, b, n):
    h = (b - a)/n
    x = np.linspace(a, b, n+1)[1:]
    return h * np.sum(f(x))
```

Gives an upper bound for increasing functions and vice versa for decreasing functions.

3.2.3 Trapezoid Method

This method averages the left and right estimates using trapezoids:

$$\int_a^b f(x)dx \approx \frac{h}{2} \left[f(a) + 2 \sum_{i=1}^{n-1} f(a + i \cdot h) + f(b) \right] \tag{51}$$

Algorithm 10 Trapezoid Integration

Require: Function f, interval $[a, b]$, number of subintervals n
Ensure: Approximation of $\int_a^b f(x)dx$
0: $h \leftarrow \frac{b-a}{n}$
0: $S \leftarrow \frac{h}{2} \cdot (f(a) + f(b))$
0: **for** $i = 1$ to $n - 1$ **do**
0: $\quad S \leftarrow S + h \cdot f(a + i \cdot h)$
0: **end for**
0: **return** S =0

Python snippet for the trapezoidal method:

```
def composite_trapezoid(f, a, b, n):
    h = (b - a)/n
```

```
    x = np.linspace(a, b, n+1)
    y = f(x)
    return h/2 * (y[0] + 2*np.sum(y[1:-1]) + y[-1])
```

Achieves second-order convergence through its linear approximation.

3.2.4 Newton-Cotes Method

The general Newton-Cotes formula for degree k is:

$$\int_a^b f(x)dx \approx \frac{h}{k!} \sum_{i=0}^{k} w_i f(a + i \cdot h) \tag{52}$$

Where w_i are coefficients derived from polynomial interpolation. For Simpson's rule (degree 2):

$$\int_a^b f(x)dx \approx \frac{h}{3} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right] \tag{53}$$

Algorithm 11 Newton-Cotes Integration

Require: Function f, interval $[a, b]$, number of subintervals n
Ensure: Approximation of $\int_a^b f(x)dx$
0: $h \leftarrow \frac{b-a}{n}$
0: $S \leftarrow 0$
0: **for** $i = 0$ to $n - 1$ **do**
0: $x_i \leftarrow a + i \cdot h$
0: $S \leftarrow S + f(x_i)$
0: **end for**
0: **Calculate divided differences**
0: **for** $k = 2$ to n **do**
0: $d_k \leftarrow 0$
0: **for** $i = 0$ to $n - k$ **do**
0: $d_k \leftarrow d_k + \binom{n-i-1}{k-1} \cdot f(x_i + (k-1) \cdot h)$
0: **end for**
0: $S \leftarrow S + \frac{h}{k!} \cdot d_k$
0: **end for**
0: **return** S =0

Python snippet for the Newton-cotes method:

```
def newton_cotes(f, a, b, n, degree):
    if degree not in [2, 3, 4]:
        raise ValueError

    num_sub = n // degree
    if num_sub < 1:
        num_sub = 1
    actual_n = num_sub * degree

```

```
    h = (b - a) / actual_n
    total = 0.0

    for i in range(num_sub):
        sub_a = a + i * degree * h
        sub_b = sub_a + degree * h
        x = np.linspace(sub_a, sub_b, degree + 1)
        y = f(x)

        if degree == 2:
            total += h/3 * (y[0] + 4*y[1] + y[2])
        elif degree == 3:
            total += 3*h/8 * (y[0] + 3*y[1] + 3*y[2] + y[3])
        elif degree == 4:
            total += 2*h/45 * (7*y[0] + 32*y[1] + 12*y[2] + 32*y[3] + 7*y[4])

    return total
```

3.2.5 Romberg Integration

This method combines Richardson extrapolation with trapezoidal estimates:

$$R_{k,j} = \frac{4^j R_{k,j-1} - R_{k-1,j-1}}{4^j - 1} \tag{54}$$

Algorithm 12 Romberg Integration

Require: Function f, interval $[a, b]$, maximum number of extrapolations K
Ensure: Approximation of $\int_a^b f(x)dx$
0: Initialize $T[K+1]$ with $T[0] = \frac{h}{2}(f(a) + f(b))$
0: **for** $k = 1$ to K **do**
0: $h \leftarrow \frac{h}{2}$
0: $T[k] \leftarrow T[k-1]/2 + h\sum_{i=0}^{2^{k-1}} f(a + (2i+1)h)$
0: **for** $j = 1$ to k **do**
0: $T[k] \leftarrow (4^j T[k] - T[k-1])/(4^j - 1)$
0: **end for**
0: **end for**
0: **return** $T[K]$ =0

Python snippet for the Romberg method:

```
def romberg(f, a, b, max_k):
    T = np.zeros(max_k + 1)
    h = b - a
    T[0] = (h / 2) * (f(a) + f(b))

    for k in range(1, max_k + 1):
        h /= 2
```

```
        x_new = a + h * np.arange(1, 2**k, 2)
        T[k] = T[k-1]/2 + h * np.sum(f(x_new))

    for j in range(1, max_k + 1):
        for k in range(j, max_k + 1):
            T[k] = (4**j * T[k] - T[k-1]) / (4**j - 1)

    return T[max_k]
```

3.2.6 Gauss-Legendre Integration

Uses optimally spaced points and weights:

$$\int_a^b f(x)dx \approx \frac{b-a}{2} \sum_{i=1}^{n} w_i f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right) \tag{55}$$

Algorithm 13 Gauss-Legendre Integration

Require: Function f, interval $[a, b]$, number of points n
Ensure: Approximation of $\int_a^b f(x)dx$
0: Compute Legendre polynomials $P_n(x)$
0: Compute roots x_i and weights w_i for $P_n(x)$
0: Transform roots and weights to interval $[a, b]$
0: $S \leftarrow 0$
0: **for** $i = 0$ to $n - 1$ **do**
0: $\quad S \leftarrow S + w_i \cdot f(x_i)$
0: **end for**
0: **return** $S \cdot \frac{b-a}{2}$ =0

Python snippet for the Gauss-Legendre method:

```
def legendre_poly(n, x):
    if n == 0:
        return np.ones_like(x)
    elif n == 1:
        return x
    else:
        return ((2*n-1)*x*legendre_poly(n-1,x) - (n-1)*legendre_poly(n-2,x))/n

def legendre_roots_weights(n):
    roots = np.zeros(n)
    weights = np.zeros(n)
    x0 = np.cos(np.pi * (np.arange(1, n+1) - 0.25) / (n + 0.5))

    for i in range(n):
        x = x0[i]
        while True:
            P, dP = legendre_poly(n, x), 0
```

```
            # Calculate derivative using recurrence
            if x != 0:
                dP = n*(legendre_poly(n-1,x) - x*legendre_poly(n,x))/(1-x**2)
            else:
                dP = n*legendre_poly(n-1,x)

            dx = P/dP
            x -= dx

        roots[i] = x
        weights[i] = 2/((1-x**2)*dP**2)

    return roots, weights

def gauss_legendre(f, a, b, n):
    x, w = legendre_roots_weights(n)
    x_trans = 0.5*(b-a)*x + 0.5*(b+a)
    w_trans = 0.5*(b-a)*w
    return np.sum(w_trans * f(x_trans))
```

3.2.7 Gauss-Chebyshev Integration

Employs weighted integration with Chebyshev polynomials:

$$\int_a^b f(x)dx \approx \frac{\pi}{n} \sum_{k=1}^{n} f\left(\frac{a+b}{2} + \frac{b-a}{2} \cos\left(\frac{2k-1}{2n}\pi\right)\right) \tag{56}$$

Algorithm 14 Gauss-Chebyshev Integration

Require: Function f, interval $[a, b]$, number of points n
Ensure: Approximation of $\int_a^b f(x)dx$
0: Compute Chebyshev polynomials $T_n(x)$
0: Compute roots x_i and weights w_i for $T_n(x)$
0: Transform roots and weights to interval $[a, b]$
0: $S \leftarrow 0$
0: **for** $i = 0$ to $n - 1$ **do**
0: $\quad S \leftarrow S + w_i \cdot f(x_i)$
0: **end for**
0: **return** $S \cdot \frac{b-a}{2}$ =0

Python snippet for the Gauss-Chebyshev method:

```
def chebyshev_poly(n):
    if n == 0:
        return [1]
    elif n == 1:
        return [1, 0]
    else:
```

```
        coeff = 2*np.pad(chebyshev_poly(n-1), (0,1), 'constant')
        coeff[:-2] -= chebyshev_poly(n-2)
        return coeff

def chebyshev_roots(n):
    return np.cos(np.pi * (2*np.arange(1, n+1) - 1) / (2*n))

def chebyshev_weights(n):
    return np.full(n, np.pi/n)

def gauss_chebyshev(f, a, b, n):
    roots = chebyshev_roots(n)
    weights = chebyshev_weights(n)

    # Transform from [-1,1] to [a,b]
    x_trans = 0.5*(b - a)*roots + 0.5*(b + a)
    w_trans = 0.5*(b - a)*weights

    # Account for the weight function
    return np.sum(w_trans * f(x_trans) * np.sqrt(1 - ((2*x_trans-(b+a))/(b-a))**2)
        )
```

3.3 Python snippet for Integration comparison

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import os

# Define various integration methods
def left_rectangular(f, a, b, n):
    h = (b - a)/n
    x = np.linspace(a, b, n+1)[:-1]
    return h * np.sum(f(x))

def right_rectangular(f, a, b, n):
    h = (b - a)/n
    x = np.linspace(a, b, n+1)[1:]
    return h * np.sum(f(x))

def composite_trapezoid(f, a, b, n):
    h = (b - a)/n
    x = np.linspace(a, b, n+1)
    y = f(x)
    return h/2 * (y[0] + 2*np.sum(y[1:-1]) + y[-1])

def newton_cotes(f, a, b, n, degree=2):
```

```
    if degree not in [2, 3, 4]:
        raise ValueError

    num_sub = n // degree
    actual_n = num_sub * degree

    h = (b - a) / actual_n
    total = 0.0

    for i in range(num_sub):
        sub_a = a + i * degree * h
        sub_b = sub_a + degree * h
        x = np.linspace(sub_a, sub_b, degree + 1)
        y = f(x)

        if degree == 2:
            total += h/3 * (y[0] + 4*y[1] + y[2])
        elif degree == 3:
            total += 3*h/8 * (y[0] + 3*y[1] + 3*y[2] + y[3])
        elif degree == 4:
            total += 2*h/45 * (7*y[0] + 32*y[1] + 12*y[2] + 32*y[3] + 7*y[4])

    return total

def romberg(f, a, b, max_k):
    T = np.zeros(max_k + 1)
    h = b - a
    T[0] = (h / 2) * (f(a) + f(b))

    for k in range(1, max_k + 1):
        h /= 2
        x_new = a + h * np.arange(1, 2**k, 2)
        T[k] = T[k-1]/2 + h * np.sum(f(x_new))

    for j in range(1, max_k + 1):
        for k in range(j, max_k + 1):
            T[k] = (4**j * T[k] - T[k-1]) / (4**j - 1)

    return T[max_k]

def gauss_legendre(f, a, b, n):
    x, w = legendre_roots_weights(n)
    x_trans = 0.5*(b-a)*x + 0.5*(b+a)
    w_trans = 0.5*(b-a)*w
    return np.sum(w_trans * f(x_trans))

def gauss_chebyshev(f, a, b, n):
```

```
    roots = chebyshev_roots(n)
    weights = chebyshev_weights(n)

    x_trans = 0.5*(b - a)*roots + 0.5*(b + a)
    w_trans = 0.5*(b - a)*weights

    return np.sum(w_trans * f(x_trans) * np.sqrt(1 - ((2*x_trans-(b+a))/(b-a))**2)
        )

# Generate results for different methods
def generate_results(f, a, b, ns):
    methods = [
        ('Left Rect', left_rectangular),
        ('Right Rect', right_rectangular),
        ('Trapezoid', composite_trapezoid),
        ('Newton-Cotes 2', lambda f, a, b, n: newton_cotes(f, a, b, n, 2)),
        ('Newton-Cotes 3', lambda f, a, b, n: newton_cotes(f, a, b, n, 3)),
        ('Newton-Cotes 4', lambda f, a, b, n: newton_cotes(f, a, b, n, 4)),
        ('Romberg', lambda f, a, b, n: romberg(f, a, b, n)),
        ('Gauss-Legendre', gauss_legendre),
        ('Gauss-Chebyshev', gauss_chebyshev)
    ]

    exact = exact_integral(a, b)

    data = []
    for n in ns:
        row = {'n': n}
        for name, method in methods:
            try:
                row[name] = method(f, a, b, n)
            except Exception as e:
                row[name] = np.nan
        data.append(row)

    results_df = pd.DataFrame(data)
    results_df['Exact'] = exact

    # Create error DataFrame
    error_data = {'n': ns}
    for name, _ in methods:
        error_data[name + '_error'] = np.abs((results_df[name] - exact)/exact)

    error_df = pd.DataFrame(error_data)
    error_df = error_df.rename(columns={c: c.replace('_error', '') for c in
        error_df.columns if c != 'n'})

```

```
    return results_df, error_df

# Example function and exact integral
def original_function(x):
    return 57.753 + (-10.779)*1e-3*x + (-11.51)*1e5/(x**2) + 5.328*1e-6*x**2

def exact_integral(a, b):
    def integral(x):
        return 57.753*x + (-10.779)*1e-3*(x**2)/2 + (-11.51)*1e5*(-1/x) + 5.328*1e
            -6*(x**3)/3
    return integral(b) - integral(a)

if __name__ == "__main__":
    a = 298
    b = 1500
    ns = np.arange(1, 21)

    results_df, error_df = generate_results(original_function, a, b, ns)

    # Plot results
    plt.figure(figsize=(10, 6))
    for col in results_df.columns:
        if col not in ['n', 'Exact']:
            plt.plot(results_df['n'], results_df[col], label=col)
    plt.plot(results_df['n'], results_df['Exact'], 'k--', label='Exact')
    plt.xlabel('n')
    plt.ylabel('Integral Value')
    plt.title('Integration Method Comparison')
    plt.legend()
    plt.grid(True)
    plt.show()

    plt.figure(figsize=(10, 6))
    for col in error_df.columns:
        if col != 'n':
            plt.plot(error_df['n'], error_df[col], label=col)
    plt.xlabel('n')
    plt.ylabel('Absolute Error')
    plt.yscale("log")
    plt.title('Integration Error Comparison')
    plt.legend()
    plt.grid(True)
    plt.show()
```

3.4 Results

The convergence behavior across methods is shown in Table 8. Figure 3.4 demonstrates the approximation quality for different n, while Figure 3.4 presents the error characteristics.

Table 8: Integration Results

n	Left Rect	Right Rect	Trapezoid	NC 2	NC 3	NC 4	Romberg	Legendre	Chebyshev	Exact
1	50,547.56	63,779.26	57,163.41	59,878.09	60,201.93	60,515.38	59,878.09	61,235.44	96,188.40	60,623.26
2	25,891.50	62,507.35	59,199.42	59,878.09	60,201.93	60,515.38	60,274.08	61,002.63	67,343.82	60,623.26
3	57,659.03	62,069.60	59,864.32	59,878.09	60,201.93	60,515.38	60,598.10	60,705.79	63,222.57	60,623.26
4	58,502.56	61,810.48	60,156.52	60,475.55	60,201.93	60,515.38	60,594.59	60,639.30	62,060.86	60,623.26
5	58,985.91	61,632.25	60,309.08	60,475.55	60,201.93	60,515.38	60,623.72	60,626.19	61,549.60	60,623.26
6	59,295.52	61,500.80	60,398.16	60,576.11	60,548.00	60,515.38	60,620.82	60,623.70	61,270.65	60,623.26
7	59,509.32	61,399.6	60,454.4	60,576.11	60,548.00	60,515.38	60,623.50	60,623.5	61,100.59	60,623.26
8	59,665.18	61,319.14	60,492.16	60,604.0	60,548.00	60,612.60	60,623.03	60,623.27	60,989.38	60,623.26
9	59,783.51	61,253.70	60,518.61	60,604.04	60,600.39	60,612.60	60,623.30	60,623.26	60,912.83	60,623.26
10	59,876.26	61,199.43	60,537.85	60,614.10	60,600.39	60,612.60	60,623.24	60,623.26	60,857.95	60,623.26
11	59,950.82	61,153.70	60,552.26	60,614.10	60,600.39	60,612.60	60,623.26	60,623.26	60,817.29	60,623.26
12	60,012.01	61,114.65	60,563.33	60,618.39	60,614.19	60,621.21	60,623.26	60,623.26	60,786.34	60,623.26
13	60,063.11	61,080.93	60,572.02	60,618.39	60,614.19	60,621.21	60,623.26	60,623.26	60,762.24	60,623.26
14	60,106.39	61,051.51	60,578.95	60,620.45	60,614.19	60,621.21	60,623.26	60,623.26	60,743.11	60,623.26
15	60,143.51	61,025.63	60,584.57	60,620.50	60,619.01	60,621.21	60,623.26	60,623.26	60,727.67	60,623.26
16	60,175.70	61,002.68	60,589.19	60,621.53	60,619.01	60,622.70	60,623.26	60,623.26	60,715.04	60,623.26
17	60,203.86	60,982.20	60,593.03	60,621.53	60,619.01	60,622.70	60,623.26	60,623.26	60,704.56	60,623.26
18	60,228.71	60,963.81	60,596.26	60,622.14	60,621.02	60,622.70	60,623.26	60,623.26	60,695.78	60,623.26
19	60,250.80	60,947.20	60,599.00	60,622.14	60,621.02	60,622.70	60,623.26	60,623.26	60,688.35	60,623.26
20	60,270.55	60,932.13	60,601.34	60,622.51	60,621.02	60,623.07	60,623.26	60,623.26	60,682.01	60,623.26

The results demonstrate that Gaussian methods achieve highest accuracy with significantly fewer points. The Romberg method shows rapid convergence through extrapolation. Newton-Cotes methods provide good balance between simplicity and accuracy. The trapezoidal rule exhibits characteristic even-order convergence behavior.

For precise calculation of CaO's enthalpy change between 298 K and 1500 K, Gaussian quadrature, especially Gauss-legendre quadrature methods are recommended for their optimal accuracy-computation trade-off. When implementing these methods in material science applications, careful consideration of error tolerance requirements and computational resources should guide method selection.

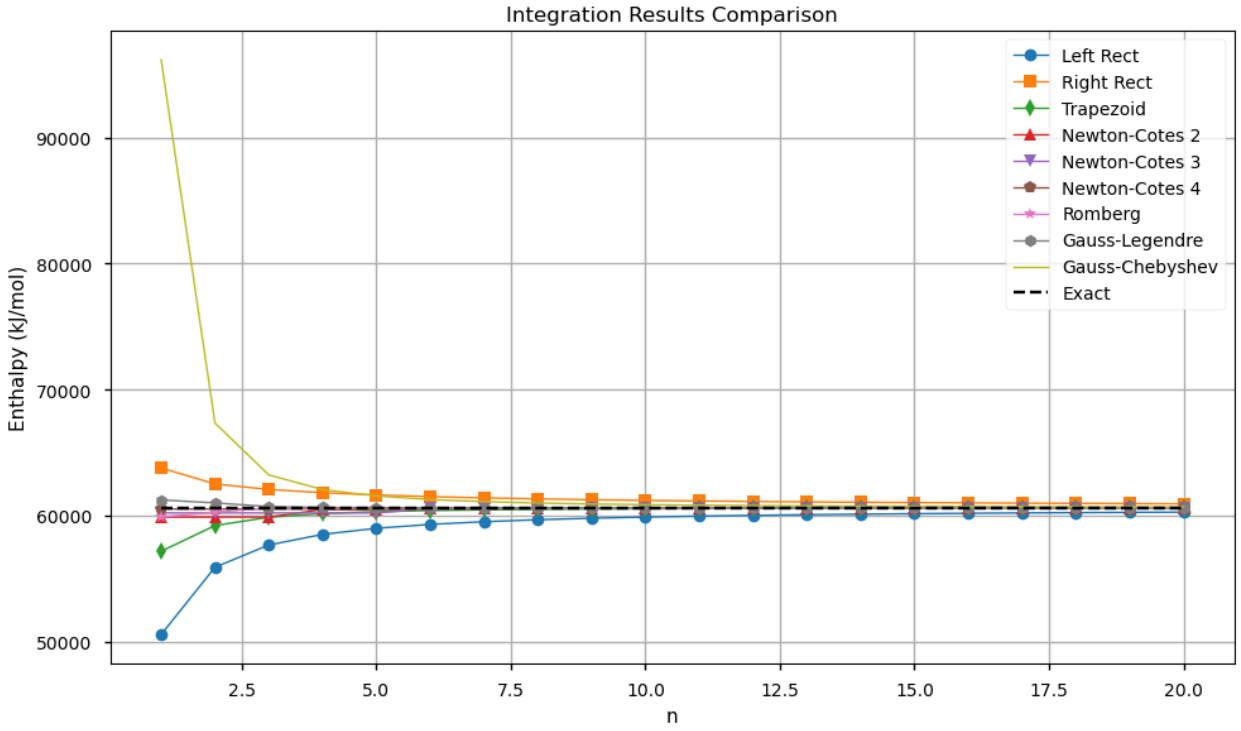


Figure 22: Approximation of Integral

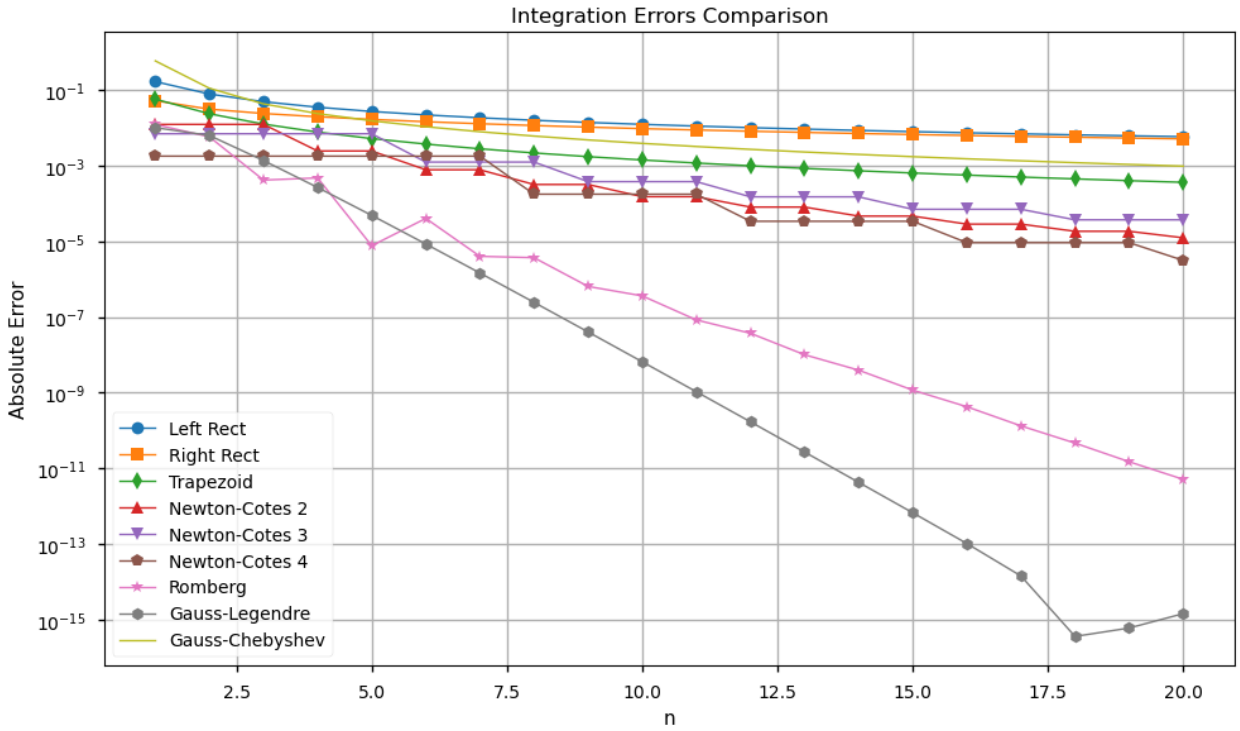


Figure 23: Error of Integral

4 Linear Systems

4.1 Real Case: Copper Smelting Material Balance

The main reaction in the Smelting Furnace is the oxidation of chalcopyrite concentrate into matte. In this stage, SiO_2 is used as a flux to capture impurities and regulate slag composition. The main reaction in the Smelting Furnace is:

$$\mathrm{CuFeS_2}(s) + \ldots \mathrm{O_2}(g) + w\mathrm{SiO_2}(s) \rightarrow 0.5\mathrm{Cu_2S} - x\mathrm{FeS}(l) + (1-x)\mathrm{FeO} - w\mathrm{SiO_2}(l) + \ldots \mathrm{SO_2}(g)$$

No chemical reactions occur in the Slag Cleaning Furnace; it only separates slag and matte by heating the molten slag and matte with electrodes in an electric furnace.

4.1.1 Assumptions for Calculations

1. Matte consists of Cu_2S and FeS.
2. Off-gas consists of N_2, SO_2, and CO_2.
3. C-slag consists of Fe_2O_3, CaO, and Cu_2O.
4. C-slag entering the S-furnace weighs 9.98 tph with 13.25% Cu and 43.47% Fe.
5. Cl-slag consists of Fe_2SiO_4, Ca_2SiO_4, SiO_2, Al_2O_3, and Cu_2O.
6. Minor elements in the concentrate, such as Au, Ag, Pb, As, Sb, Zn, are negligible. Au and Ag are carried to the final copper product and separated in anode slime, while other minor elements are assumed to go to slag.

4.1.2 Mass balance equations with known information

1. Copper Balance
$$-0.346w_{\mathrm{CuFeS_2}} + 0.799w_{\mathrm{Cu_2S}} + 0.888w_{\mathrm{Cu_2O}} = 1.325 \tag{57}$$

2. Iron Balance
$$-0.304w_{\mathrm{CuFeS_2}} - 0.466w_{\mathrm{FeS_2}} + 0.635w_{\mathrm{FeS}} + 0.548w_{\mathrm{Fe_2SiO_4}} = 4.347 \tag{58}$$

3. Sulfur Balance
$$-0.349w_{\mathrm{CuFeS_2}} - 0.535w_{\mathrm{FeS_2}} + 0.202w_{\mathrm{Cu_2S}} + 0.365w_{\mathrm{FeS}} + 0.501w_{\mathrm{SO_2}} = 0 \tag{59}$$

4. Oxygen Balance
$$-w_{\mathrm{O_2}}(\mathrm{blast}) + 0.157w_{\mathrm{Fe_2SiO_4}} + 0.112w_{\mathrm{Cu_2O}} + 0.500w_{\mathrm{SO_2}} + 0.727w_{\mathrm{CO_2}} = 2.035 \tag{60}$$

5. Carbon Balance
$$-w_{\mathrm{fuel}} + 0.273w_{\mathrm{CO_2}} = 0 \tag{61}$$

6. SiO_2 Balance

$$-w_{\text{flux}} + 0.295w_{Fe_2SiO_4} + 0.349w_{Ca_2SiO_4} + w_{SiO_2}(\text{cl-slag}) = 17.904 \tag{62}$$

7. CaO Balance

$$0.651w_{Ca_2SiO_4} = 4.146 \tag{63}$$

8. Al_2O_3 Balance

$$w_{Al_2O_3}(\text{cl-slag}) = 3.704 \tag{64}$$

9. Matte Grade

$$0.68w_{FeS} - 0.119w_{Cu_2S} = 0 \tag{65}$$

10. Fe/SiO_2 in Slag

$$0.241w_{Fe_2SiO_4}(\text{cl-slag}) - 0.363w_{Ca_2SiO_4}(\text{cl-slag}) - 1.040w_{SiO_2}(\text{cl-slag}) = 0 \tag{66}$$

11. Cu in Slag

$$0.879w_{Cu_2O}(\text{cl-slag}) - 0.009w_{Fe_2SiO_4}(\text{cl-slag}) - 0.009w_{Ca_2SiO_4}(\text{cl-slag}) - 0.009w_{SiO_2}(\text{cl-slag}) = 0 \tag{67}$$

12. Weight of Sulfide Minerals in Concentrate

$$w_{CuFeS_2} + w_{FeS_2} = 100.013 \tag{68}$$

13. $CuFeS_2/FeS_2$ in Concentrate

$$0.150w_{CuFeS_2} - 0.85w_{FeS_2} = 0 \tag{69}$$

14. Weight of C-Slag

$$w_{\text{C-slag}} = 10 \tag{70}$$

15. Weight of Fuel

$$w_{\text{fuel}} = 1.235 \tag{71}$$

16. Total N_2

$$w_{N_2} = 76.64 \tag{72}$$

$$\mathbf{A} = \begin{bmatrix}
-0.35 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.80 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.89 & 0.00 & 0.00 \\
-0.30 & -0.47 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.64 & 0.55 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
-0.35 & -0.54 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.20 & 0.37 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.50 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & -1.00 & 0.00 & 0.00 & 0.00 & 0.16 & 0.00 & 0.00 & 0.00 & 0.11 & 0.50 & 0.73 \\
0.00 & 0.00 & 0.00 & 0.00 & -1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.27 \\
0.00 & 0.00 & 0.00 & -1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.30 & 1.00 & 0.35 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.65 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & -0.12 & 0.68 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.24 & -1.04 & -0.36 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & -0.01 & -0.01 & -0.01 & 0.00 & 0.88 & 0.00 & 0.00 \\
1.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.15 & -0.85 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00
\end{bmatrix}$$

$$\mathbf{b^T} = \begin{bmatrix} 1.33 & 4.35 & 0.00 & 2.04 & 0.00 & 17.90 & 4.14 & 3.70 & 0.00 & 0.00 & 0.00 & 100.01 & 0.00 & 10.00 & 1.24 & 76.64 \end{bmatrix}$$

$$\mathbf{x^T} = \begin{bmatrix} w_{\mathrm{CuFeS_2}} & w_{\mathrm{FeS_2}} & w_{\text{C-Slag}} & w_{\mathrm{Flux}} & w_{\mathrm{Fuel}} & w_{\mathrm{O_2}} & w_{\mathrm{N_2}} & w_{\mathrm{Cu_2S}} & w_{\mathrm{FeS}} & w_{\mathrm{Fe_2SiO_4}} & w_{\mathrm{SiO_2}} & w_{\mathrm{Ca_2SiO_4}} & w_{\mathrm{Al_2O_3}} & w_{\mathrm{Cu_2O}} & w_{\mathrm{SO_2}} & w_{\mathrm{CO_2}} \end{bmatrix}$$

A linear system is a set of linear equations that can be written in matrix form as:

$$A \cdot \mathbf{x} = \mathbf{b} \tag{73}$$

where A is the coefficient matrix, $\mathbf{x}$ is the vector of unknowns, and $\mathbf{b}$ is the vector of constants.

4.2 Methods

4.2.1 Jacobian Method

The Jacobi method is an iterative method for solving a linear system of equations. The algorithm is as follows:

Algorithm 15 Jacobi Method

$\mathbf{x}^{(0)}$, an initial guess for the solution vector
for $k = 0$ to $max\_iterations$ **do**
  for $i = 0$ to $n - 1$ **do**
    $x_i^{(k+1)} \leftarrow \frac{\mathbf{b}_i - \cdot \sum_{j \neq i} A_{ij} x_j^{(k)}}{A_{ii}}$;
  end for
  return $\mathbf{x}^{(k+1)}$;

Python snippet for the Jacobian method:

```
def jacobi(A, b, max_iterations):
    n = len(b)
    x = np.zeros_like(b, dtype=np.float64)
    results = []
    results.append({'k': 0, 'x': x.copy(), 'residual': np.linalg.norm(A @ x - b)})

    for k in range(max_iterations):
        x_new = np.zeros_like(x)
        for i in range(n):
            sum_total = np.dot(A[i, :], x) - A[i, i] * x[i]
            x_new[i] = (b[i] - sum_total) / A[i, i]
        x = x_new.copy()
        residual = np.linalg.norm(A @ x - b)
        results.append({'k': k + 1, 'x': x.copy(), 'residual': residual})

    return pd.DataFrame(results)
```

4.2.2 Gauss-Seidel Method

The Gauss-Seidel method is another iterative method for solving a linear system. The algorithm is as follows:

Algorithm 16 Gauss-Seidel Method

$\mathbf{x}^{(0)}$, an initial guess for the solution vector
for $k = 0$ to $max\_iterations$ **do**
  for $i = 0$ to $n - 1$ **do**
    $s \leftarrow \sum_{j=0}^{i-1} A_{ij} x_j^{(k)}$;
    $t \leftarrow \sum_{j=i+1}^{n} A_{ij} x_j^{(k)}$;
    $x_i^{(k+1)} \leftarrow \frac{\mathbf{b}_i - s - t}{A_{ii}}$;
  end for
  return $\mathbf{x}^{(k+1)}$;

Python snippet for the Gauss-Seidel method:

```
def gauss_seidel(A, b, max_iterations):
    n = len(b)
    x = np.zeros_like(b, dtype=np.float64)
    results = []
    results.append({'k': 0, 'x': x.copy(), 'residual': np.linalg.norm(A @ x - b)})

    for k in range(max_iterations):
        x_new = np.zeros_like(x)
        for i in range(n):
            sum_before = np.dot(A[i, :i], x_new[:i])
            sum_after = np.dot(A[i, i+1:], x[i+1:])
            x_new[i] = (b[i] - sum_before - sum_after) / A[i, i]
        x = x_new.copy()
        residual = np.linalg.norm(A @ x - b)
        results.append({'k': k + 1, 'x': x.copy(), 'residual': residual})

    return pd.DataFrame(results)
```

4.2.3 SOR Method

The SOR (Successive Over-Relaxation) method is an iterative method for solving a linear system. The algorithm is as follows:

Algorithm 17 SOR Method

$\mathbf{x}^{(0)}$, an initial guess for the solution vector
for $k = 0$ to $max\_iterations$ **do**
  for $i = 0$ to $n - 1$ **do**
    $w \leftarrow \mathbf{b}_i - \cdot \sum_{j=0}^{i-1} A_{ij} x_j^{(k)}$;
    $u \leftarrow \mathbf{b}_i - \cdot \sum_{j=i+1}^{n} A_{ij} x_j^{(k)}$;
    $x_i^{(k+1)} \leftarrow (1 - w) x_i^{(k)} + w$;
  end for
  return $\mathbf{x}^{(k+1)}$;

Python snippet for the SOR method:

```python
def SOR(A, b, max_iterations, w):
    n = len(b)
    x = np.zeros_like(b, dtype=np.float64)
    results = []
    results.append({'k': 0, 'x': x.copy(), 'residual': np.linalg.norm(A @ x - b)})

    for k in range(max_iterations):
        x_new = np.zeros_like(x)
        for i in range(n):
            sum_before = np.dot(A[i, :i], x_new[:i])
            sum_after = np.dot(A[i, i+1:], x[i+1:])
            x_new[i] = (1 - w) * x[i] + w * (b[i] - sum_before - sum_after) / A[i,
                i]
        x = x_new.copy()
        residual = np.linalg.norm(A @ x - b)
        results.append({'k': k + 1, 'x': x.copy(), 'residual': residual})

    return pd.DataFrame(results)
```

4.2.4 Steepest Descent Method

The Steepest Descent method is an iterative method for solving a linear system. The algorithm is as follows:

Algorithm 18 Steepest Descent Method

$\mathbf{x}^{(0)}$, an initial guess for the solution vector
$\mathbf{r}^{(0)} \leftarrow \mathbf{b} - A \cdot \mathbf{x}^{(0)}$;
$\mathbf{residuals}^{(0)} \leftarrow \|\mathbf{r}^{(0)}\|$;
for $k = 1$ to $max\_iterations$ **do**
    $\mathbf{Ar} \leftarrow A \cdot \mathbf{r}^{(k-1)}$;
    $\alpha \leftarrow \frac{\mathbf{r}^{(k-1)} \cdot \mathbf{r}^{(k-1)}}{\mathbf{r}^{(k-1)} \cdot \mathbf{Ar}^{(k-1)}}$;
    $\mathbf{x}^{(k)} \leftarrow \mathbf{x}^{(k-1)} + \alpha \cdot \mathbf{r}^{(k-1)}$;
    $\mathbf{r}^{(k)} \leftarrow \mathbf{r}^{(k-1)} - \alpha \cdot \mathbf{Ar}^{(k-1)}$;
    $\mathbf{residuals}^{(k)} \leftarrow \|\mathbf{r}^{(k)}\|$;
end for
return $\mathbf{x}^{(k)}$; $=0$

Python snippet for the Steepest Descent method:

```python
def steepest_descent(A, b, max_iterations):
    x = np.zeros_like(b, dtype=np.float64)
    r = b - A @ x
    residuals = [np.linalg.norm(r)]
    results = []
    results.append({
        'k': 0,
        'x': x.copy(),
        'p': r.copy(),
```

```
        'alpha': np.nan,
        'residual': residuals[0]
    })

    for k in range(max_iterations):
        Ar = A @ r
        alpha = np.dot(r, r) / np.dot(r, Ar)
        x = x + alpha * r
        r = r - alpha * Ar
        residual = np.linalg.norm(r)
        residuals.append(residual)
        results.append({
            'k': k + 1,
            'x': x.copy(),
            'p': r.copy(),
            'alpha': alpha,
            'residual': residual
        })

    return pd.DataFrame(results)
```

4.2.5 Conjugate Gradient Method

The Conjugate Gradient method is an iterative method for solving a linear system. The algorithm is as follows:

Algorithm 19 Conjugate Gradient Method

$\mathbf{x}^{(0)}$, an initial guess for the solution vector
$\mathbf{r}^{(0)} \leftarrow \mathbf{b} - A \cdot \mathbf{x}^{(0)}$;
$\mathbf{p}^{(0)} \leftarrow \mathbf{r}^{(0)}$;
for $k = 1$ to $max\_iterations$ **do**
  $\mathbf{Ap} \leftarrow A \cdot \mathbf{p}^{(k-1)}$;
  $\alpha \leftarrow \frac{\mathbf{r}^{(k-1)} \cdot \mathbf{r}^{(k-1)}}{\mathbf{r}^{(k-1)} \cdot \mathbf{Ap}^{(k-1)}}$;
  $\mathbf{x}^{(k)} \leftarrow \mathbf{x}^{(k-1)} + \alpha \cdot \mathbf{p}^{(k-1)}$;
  $\mathbf{r}^{(k)} \leftarrow \mathbf{r}^{(k-1)} - \alpha \cdot \mathbf{Ap}^{(k-1)}$;
  $\mathbf{beta} \leftarrow \frac{\mathbf{r}^{(k)} \cdot \mathbf{r}^{(k)}}{\mathbf{r}^{(k-1)} \cdot \mathbf{r}^{(k-1)}}$;
  $\mathbf{p}^{(k)} \leftarrow \mathbf{r}^{(k)} + \beta \cdot \mathbf{p}^{(k-1)}$;
end for
return $\mathbf{x}^{(k)}$; =0

Python snippet for the Conjugate Gradient method:

```
def conjugate_gradient(A, b, max_iterations):
    x = np.zeros_like(b, dtype=np.float64)
    r = b - A @ x
    p = r.copy()
    residuals = [np.linalg.norm(r)]
    results = []
```

```
    results.append({
        'k': 0,
        'x': x.copy(),
        'p': p.copy(),
        'r': r.copy(),
        'alpha': np.nan,
        'beta': np.nan,
        'residual': residuals[0]
    })

    for k in range(max_iterations):
        Ap = A @ p
        alpha = np.dot(r, r) / np.dot(p, Ap)
        x = x + alpha * p
        r_new = r - alpha * Ap
        residual = np.linalg.norm(r_new)
        residuals.append(residual)
        beta = np.dot(r_new, r_new) / np.dot(r, r)
        p = r_new + beta * p
        results.append({
            'k': k + 1,
            'x': x.copy(),
            'p': p.copy(),
            'r': r_new.copy(),
            'alpha': alpha,
            'beta': beta,
            'residual': residual
        })
        r = r_new

    return pd.DataFrame(results)
```

4.3 Python snippet for various method comparison

```
\begin{lstlisting}[style=custompython]
import numpy as np
import pandas as pd
import os
from scipy.optimize import linear_sum_assignment
import matplotlib.pyplot as plt

# Matrix preprocessing to create diagonally dominant matrix
def make_diagonally_dominant(A, b):
    n = len(b)
    A_new = A.copy()
    b_new = b.copy()
    col_order = np.arange(n)
```

```
784
785     for i in range(n):
786         if A_new[i, i] == 0:
787             for j in range(i + 1, n):
788                 if A_new[j, i] != 0:
789                     A_new[[i, j]] = A_new[[j, i]]
790                     b_new[[i, j]] = b_new[[j, i]]
791                     break
792             for k in range(i + 1, n):
793                 if A_new[i, k] != 0:
794                     A_new[:, [i, k]] = A_new[:, [k, i]]
795                     col_order[[i, k]] = col_order[[k, i]]
796                     break
797
798     cost = -np.abs(A_new)
799     row_ind, col_ind = linear_sum_assignment(cost)
800     A_new = A_new[row_ind][:, col_ind]
801     b_new = b_new[row_ind]
802     col_order = col_order[col_ind]
803
804     return A_new, b_new, col_order
805
806 # Jacobi method
807 def jacobi(A, b, max_iterations):
808     n = len(b)
809     x = np.zeros_like(b, dtype=np.float64)
810     results = []
811     results.append({'k': 0, 'x': x.copy(), 'residual': np.linalg.norm(A @ x - b)})
812
813     for k in range(max_iterations):
814         x_new = np.zeros_like(x)
815         for i in range(n):
816             sum_total = np.dot(A[i, :], x) - A[i, i] * x[i]
817             x_new[i] = (b[i] - sum_total) / A[i, i]
818         x = x_new.copy()
819         residual = np.linalg.norm(A @ x - b)
820         results.append({'k': k + 1, 'x': x.copy(), 'residual': residual})
821
822     return pd.DataFrame(results)
823
824 # Gauss-Seidel method
825 def gauss_seidel(A, b, max_iterations):
826     n = len(b)
827     x = np.zeros_like(b, dtype=np.float64)
828     results = []
829     results.append({'k': 0, 'x': x.copy(), 'residual': np.linalg.norm(A @ x - b)})
830
```

```
    for k in range(max_iterations):
        x_new = np.zeros_like(x)
        for i in range(n):
            sum_before = np.dot(A[i, :i], x_new[:i])
            sum_after = np.dot(A[i, i+1:], x[i+1:])
            x_new[i] = (b[i] - sum_before - sum_after) / A[i, i]
        x = x_new.copy()
        residual = np.linalg.norm(A @ x - b)
        results.append({'k': k + 1, 'x': x.copy(), 'residual': residual})

    return pd.DataFrame(results)

# SOR method
def SOR(A, b, max_iterations, w):
    n = len(b)
    x = np.zeros_like(b, dtype=np.float64)
    results = []
    results.append({'k': 0, 'x': x.copy(), 'residual': np.linalg.norm(A @ x - b)})

    for k in range(max_iterations):
        x_new = np.zeros_like(x)
        for i in range(n):
            sum_before = np.dot(A[i, :i], x_new[:i])
            sum_after = np.dot(A[i, i+1:], x[i+1:])
            x_new[i] = (1 - w) * x[i] + w * (b[i] - sum_before - sum_after) / A[i,
                i]
        x = x_new.copy()
        residual = np.linalg.norm(A @ x - b)
        results.append({'k': k + 1, 'x': x.copy(), 'residual': residual})

    return pd.DataFrame(results)

# Steepest Descent method
def steepest_descent(A, b, max_iterations):
    x = np.zeros_like(b, dtype=np.float64)
    r = b - A @ x
    residuals = [np.linalg.norm(r)]
    results = []
    results.append({
        'k': 0,
        'x': x.copy(),
        'p': r.copy(),
        'alpha': np.nan,
        'residual': residuals[0]
    })

    for k in range(max_iterations):
```

```
        Ar = A @ r
        alpha = np.dot(r, r) / np.dot(r, Ar)
        x = x + alpha * r
        r = r - alpha * Ar
        residual = np.linalg.norm(r)
        residuals.append(residual)
        results.append({
            'k': k + 1,
            'x': x.copy(),
            'p': r.copy(),
            'alpha': alpha,
            'residual': residual
        })

    return pd.DataFrame(results)

# Conjugate Gradient method
def conjugate_gradient(A, b, max_iterations):
    x = np.zeros_like(b, dtype=np.float64)
    r = b - A @ x
    p = r.copy()
    residuals = [np.linalg.norm(r)]
    results = []
    results.append({
        'k': 0,
        'x': x.copy(),
        'p': p.copy(),
        'r': r.copy(),
        'alpha': np.nan,
        'beta': np.nan,
        'residual': residuals[0]
    })

    for k in range(max_iterations):
        Ap = A @ p
        alpha = np.dot(r, r) / np.dot(p, Ap)
        x = x + alpha * p
        r_new = r - alpha * Ap
        residual = np.linalg.norm(r_new)
        residuals.append(residual)
        beta = np.dot(r_new, r_new) / np.dot(r, r)
        p = r_new + beta * p
        results.append({
            'k': k + 1,
            'x': x.copy(),
            'p': p.copy(),
            'r': r_new.copy(),
```

```
            'alpha': alpha,
            'beta': beta,
            'residual': residual
        })
        r = r_new

    return pd.DataFrame(results)

# Matrix and vector definitions
A = np.array([...])  # Matrix definition
b = np.array([...])  # Vector definition
variables = [...]     # Variable names

# Parameters
w = 0.965
max_iterations = 10

# Preprocessing
A_new, b_new, col_order = make_diagonally_dominant(A, b)
inv_col_order = np.argsort(col_order)

# Run methods
jacob_result = jacobi(A_new, b_new, max_iterations)
gs_result = gauss_seidel(A_new, b_new, max_iterations)
sor_result = SOR(A_new, b_new, max_iterations, w)
sd_result = steepest_descent(A, b, max_iterations)
cg_result = conjugate_gradient(A, b, max_iterations)

# Process and save results
output_dir = "06_linearsys/results"
os.makedirs(output_dir, exist_ok=True)

with pd.ExcelWriter(os.path.join(output_dir, "linear_system_results.xlsx")) as
    writer:
    jacob_result.to_excel(writer, sheet_name='Jacobi', index=False)
    gs_result.to_excel(writer, sheet_name='Gauss-Seidel', index=False)
    sor_result.to_excel(writer, sheet_name='SOR', index=False)
    sd_result.to_excel(writer, sheet_name='Steepest-Descent', index=False)
    cg_result.to_excel(writer, sheet_name='Conjugate-Gradient', index=False)

# Plot residuals comparison
def plot_residuals_comparison(error_df, output_dir):
    markerss = ['o', 's', 'd', '^', 'v', 'p', '*', 'h', '+', 'x']
    plt.figure(figsize=(10, 6))
    plt.style.use('seaborn-v0_8-notebook')
    for i, column in enumerate(error_df.columns):
```

```
        plt.semilogy(error_df.index, error_df[column], marker=markerss[i], label=
            column)
    plt.title('Residuals Comparison of Different Methods')
    plt.xlabel('Iteration')
    plt.ylabel('Residual')
    plt.legend()
    plt.grid(True)
    plt.savefig(os.path.join(output_dir, "residuals_comparison.png"))
    plt.show()

# Generate and display residuals comparison
error = pd.DataFrame({
    'Jacobi': jacob_result['residual'],
    'Gauss-Seidel': gs_result['residual'],
    'SOR': sor_result['residual'],
    'Steepest-Descent': sd_result['residual'],
    'Conjugate-Gradient': cg_result['residual']
})
error.index = jacob_result['k']

print("Residuals Comparison:")
print(error.to_string())
plot_residuals_comparison(error, output_dir)
```

4.4 Results

4.4.1 Jacobian Method

Table 9: Results of Jacobian method (Part 1)

k	w_{CuFeS2}	w_{FeS2}	$w_{\text{C\_Slag}}$	w_{Flux}	w_{Fuel}	w_{O2}	w_{N2}	w_{Cu2S}	w_{FeS}
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	100.0130	0.0000	10.0000	-17.9040	1.2350	-2.0370	76.6400	1.6583	0.0000
2	100.0130	17.6494	10.0000	-13.3429	1.2350	-0.7916	76.6400	44.9681	0.2902
3	82.3636	17.6494	10.0000	2.6411	1.2350	45.7248	76.6400	44.8056	7.8694
4	82.3636	14.5348	10.0000	19.8262	1.2350	48.6781	76.6400	36.5364	7.8410
5	85.4782	14.5348	10.0000	17.7470	1.2350	36.9182	76.6400	36.2235	6.3939
6	85.4782	15.0844	10.0000	12.6714	1.2350	36.5046	76.6400	37.7447	6.3391
7	84.9286	15.0844	10.0000	13.0697	1.2350	38.7062	76.6400	37.8234	6.6053
8	84.9286	14.9874	10.0000	14.0153	1.2350	38.7995	76.6400	37.5535	6.6191
9	85.0256	14.9874	10.0000	13.9573	1.2350	38.4005	76.6400	37.5385	6.5719
10	85.0256	15.0045	10.0000	13.7861	1.2350	38.3820	76.6400	37.5861	6.5692

Table 10: Results of Jacobian method (Part 2)

k	$w_{Fe2SiO4}$	w_{SiO2}	$w_{Ca2SiO4}$	w_{Al2O3}	w_{Cu2O}	w_{SO2}	w_{CO2}	Residual
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	127.8830
1	7.9325	0.0000	6.3641	3.7040	0.0000	0.0000	0.0000	59.7167
2	63.4141	-0.3831	6.3641	3.7040	0.1462	69.0011	4.5238	54.7847
3	78.0863	12.4737	6.3641	3.7040	0.7097	70.1746	4.5238	23.4513
4	59.5129	15.8737	6.3641	3.7040	0.9913	52.4237	4.5238	13.2461
5	56.8973	11.5697	6.3641	3.7040	0.8361	52.4525	4.5238	5.8591
6	60.3020	10.9636	6.3641	3.7040	0.7653	55.8026	4.5238	2.4705
7	60.8328	11.7525	6.3641	3.7040	0.7939	55.8161	4.5238	1.0856
8	60.2194	11.8755	6.3641	3.7040	0.8074	55.2075	4.5238	0.4449
9	60.1210	11.7334	6.3641	3.7040	0.8024	55.2027	4.5238	0.1958
10	60.2295	11.7106	6.3641	3.7040	0.7999	55.3107	4.5238	0.0787

4.4.2 Gauss-Seidel Method

Table 11: Results of Gauss-Seidel method (Part 1)

k	w_{CuFeS2}	w_{FeS2}	w_{C_Slag}	w_{Flux}	w_{Fuel}	w_{O2}	w_{N2}	w_{Cu2S}	w_{FeS}
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	100.0130	17.6494	10.0000	-15.5639	1.2350	-0.7916	76.6400	1.6583	0.2902
2	82.3636	14.5348	10.0000	9.1907	1.2350	13.0825	76.6400	44.8570	7.8499
3	85.4782	15.0844	10.0000	16.9724	1.2350	42.6538	76.6400	36.1849	6.3323
4	84.9286	14.9874	10.0000	13.2262	1.2350	37.7355	76.6400	37.8304	6.6203
5	85.0256	15.0045	10.0000	13.9297	1.2350	38.5695	76.6400	37.5370	6.5690
6	85.0085	15.0015	10.0000	13.8003	1.2350	38.4232	76.6400	37.5891	6.5781
7	85.0115	15.0020	10.0000	13.8232	1.2350	38.4489	76.6400	37.5799	6.5765
8	85.0110	15.0019	10.0000	13.8192	1.2350	38.4443	76.6400	37.5816	6.5768
9	85.0111	15.0020	10.0000	13.8199	1.2350	38.4451	76.6400	37.5813	6.5767
10	85.0110	15.0020	10.0000	13.8198	1.2350	38.4450	76.6400	37.5813	6.5767

Table 12: Results of Gauss-Seidel method (Part 2)

k	$w_{Fe2SiO4}$	w_{SiO2}	$w_{Ca2SiO4}$	w_{Al2O3}	w_{Cu2O}	w_{SO2}	w_{CO2}	Residual
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	127.8830
1	7.9325	1.8382	6.3641	3.7040	0.0999	-0.8801	0.0000	70.5052
2	78.0863	15.8737	6.3641	3.7040	1.0260	64.7117	4.5238	39.1574
3	56.8869	10.9611	6.3641	3.7040	0.7590	53.6933	4.5238	7.9654
4	60.8406	11.8773	6.3641	3.7040	0.8088	55.5766	4.5238	1.4201
5	60.1196	11.7103	6.3641	3.7040	0.7997	55.2459	4.5238	0.2538
6	60.2474	11.7399	6.3641	3.7040	0.8013	55.3041	4.5238	0.0448
7	60.2248	11.7346	6.3641	3.7040	0.8010	55.2938	4.5238	0.0079
8	60.2288	11.7356	6.3641	3.7040	0.8011	55.2956	4.5238	0.0014
9	60.2281	11.7354	6.3641	3.7040	0.8011	55.2953	4.5238	0.0002
10	60.2282	11.7354	6.3641	3.7040	0.8011	55.2954	4.5238	0.0000

4.4.3 SOR Method

Table 13: Results of SOR method (Part 1)

k	w_{CuFeS2}	w_{FeS2}	$w_{\text{C\_Slag}}$	w_{Flux}	w_{Fuel}	w_{O2}	w_{N2}	w_{Cu2S}	w_{FeS}
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	96.5125	16.4355	9.6500	-15.0982	1.1918	-0.8060	73.9576	1.6003	0.2702
2	84.0302	14.8851	9.9878	6.6312	1.2335	11.6050	76.5461	41.8883	7.0833
3	85.0895	15.0112	9.9996	15.7936	1.2349	39.9094	76.6367	37.1916	6.5286
4	85.0049	15.0012	9.9999	13.8372	1.2350	38.3083	76.6399	37.6047	6.5790
5	85.0115	15.0020	10.0000	13.8335	1.2350	38.4577	76.6400	37.5787	6.5764
6	85.0110	15.0019	10.0000	13.8201	1.2350	38.4444	76.6400	37.5814	6.5767
7	85.0111	15.0020	10.0000	13.8199	1.2350	38.4451	76.6400	37.5813	6.5767
8	85.0110	15.0020	10.0000	13.8198	1.2350	38.4450	76.6400	37.5813	6.5767
9	85.0111	15.0020	10.0000	13.8198	1.2350	38.4450	76.6400	37.5813	6.5767
10	85.0110	15.0020	10.0000	13.8198	1.2350	38.4450	76.6400	37.5813	6.5767

Table 14: Results of SOR method (Part 2)

k	w_{Fe2SiO4}	w_{SiO2}	w_{Ca2SiO4}	w_{Al2O3}	w_{Cu2O}	w_{SO2}	w_{CO2}	Residual
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	127.8830
1	7.6548	1.7118	6.1413	3.5744	0.0924	-0.8126	0.0000	66.8977
2	72.7735	14.2650	6.3563	3.6995	0.9229	60.5085	4.2127	35.2671
3	59.4798	11.6592	6.3638	3.7038	0.7971	54.8835	4.5076	2.9772
4	60.3054	11.7501	6.3640	3.7040	0.8018	55.3325	4.5231	0.1778
5	60.2244	11.7351	6.3641	3.7040	0.8011	55.2930	4.5238	0.0213
6	60.2288	11.7355	6.3641	3.7040	0.8011	55.2956	4.5238	0.0009
7	60.2282	11.7354	6.3641	3.7040	0.8011	55.2953	4.5238	0.0002
8	60.2282	11.7354	6.3641	3.7040	0.8011	55.2953	4.5238	0.0000
9	60.2282	11.7354	6.3641	3.7040	0.8011	55.2953	4.5238	0.0000
10	60.2282	11.7354	6.3641	3.7040	0.8011	55.2953	4.5238	0.0000

4.4.4 Steepest Descent Method

Table 15: Results of Steepest Descent method (Part 1)

k	w_{CuFeS2}	w_{FeS2}	$w_{\text{C\_Slag}}$	w_{Flux}	w_{Fuel}	w_{O2}
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	1.19×10^{1}	3.89×10^{1}	0.0000	1.82×10^{1}	0.0000	1.60×10^{2}
2	2.67×10^{2}	-2.73×10^{1}	-3.23×10^{1}	9.12×10^{2}	4.75×10^{2}	8.61×10^{2}
3	1.79×10^{2}	-2.65×10^{3}	-3.95×10^{2}	-1.84×10^{3}	-1.08×10^{3}	-2.72×10^{3}
4	-4.03×10^{3}	-1.20×10^{4}	2.01×10^{4}	7.20×10^{4}	2.56×10^{4}	1.05×10^{4}
5	-2.13×10^{3}	4.62×10^{3}	2.97×10^{3}	2.96×10^{4}	7.80×10^{4}	3.19×10^{5}

Table 16: Results of Steepest Descent method (Part 2)

k	w_{Cu2S}	w_{FeS}	w_{Fe2SiO4}	w_{SiO2}	w_{Ca2SiO4}	w_{Al2O3}
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	3.31×10^{1}	0.0000	0.0000	0.0000	8.95×10^{2}	0.0000
2	2.37×10^{1}	-1.00×10^{1}	1.79×10^{2}	7.70×10^{2}	-7.94×10^{1}	6.41×10^{1}
3	-3.87×10^{2}	-5.76×10^{1}	1.46×10^{3}	2.33×10^{2}	-1.45×10^{2}	2.35×10^{3}
4	1.54×10^{3}	1.90×10^{-1}	-2.02×10^{4}	1.94×10^{4}	-3.55×10^{3}	-6.77×10^{3}
5	-6.83×10^{4}	6.61×10^{2}	3.79×10^{4}	-1.52×10^{4}	-7.58×10^{4}	-9.89×10^{4}

Table 17: Results of Steepest Descent method (Part 3)

k	w_{SO2}	w_{CO2}	α	β	Residual
0	0.0000	0.0000			1.28×10^{2}
1	1.10×10^{1}	6.86×10^{2}	8.95×10^{0}		8.34×10^{2}
2	-4.08×10^{2}	-6.78×10^{1}	-4.08×10^{2}	5.97×10^{-1}	6.45×10^{2}
3	7.59×10^{1}	2.52×10^{2}	2.52×10^{2}	1.99×10^{-1}	2.88×10^{2}
4	-1.47×10^{4}	5.00×10^{3}	-2.44×10^{3}	-1.19×10^{2}	3.01×10^{4}
5	1.54×10^{4}	-4.45×10^{3}	2.52×10^{3}	1.16×10^{-2}	3.11×10^{4}

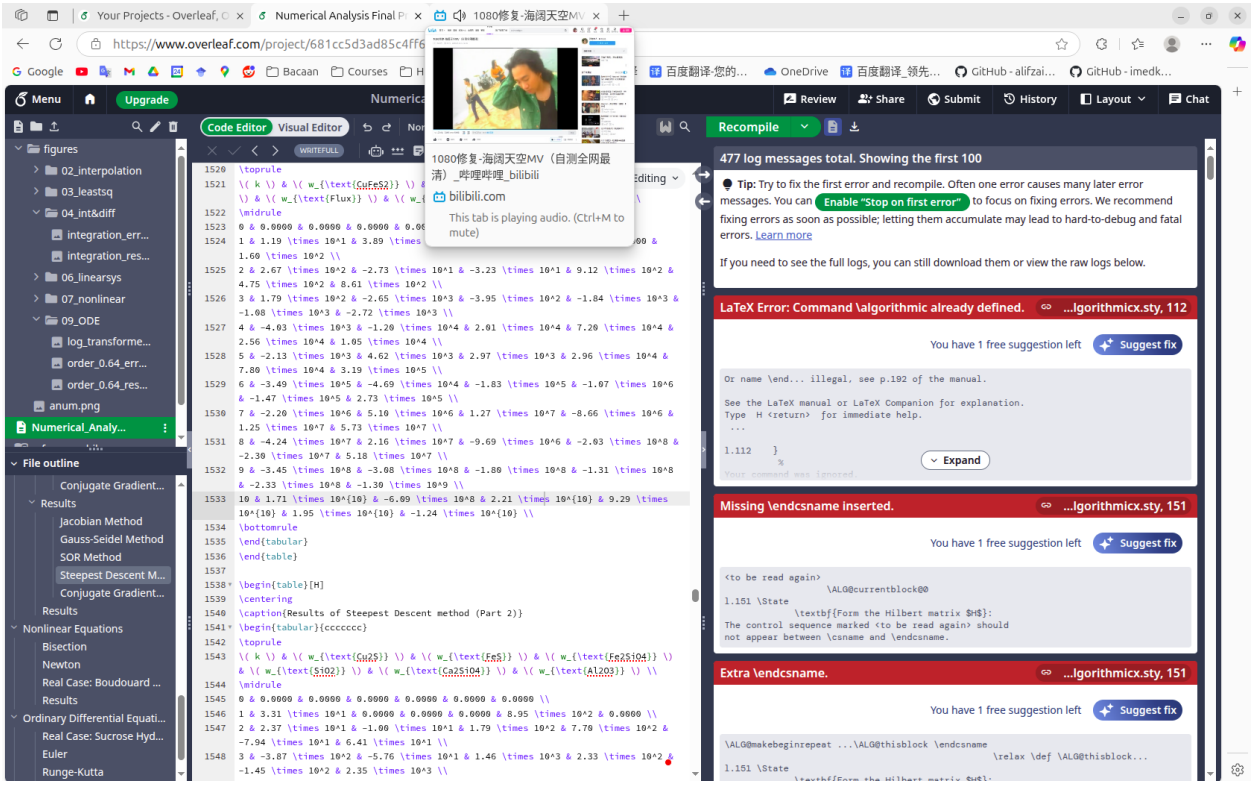


Figure 24: Unable to compile due to large number

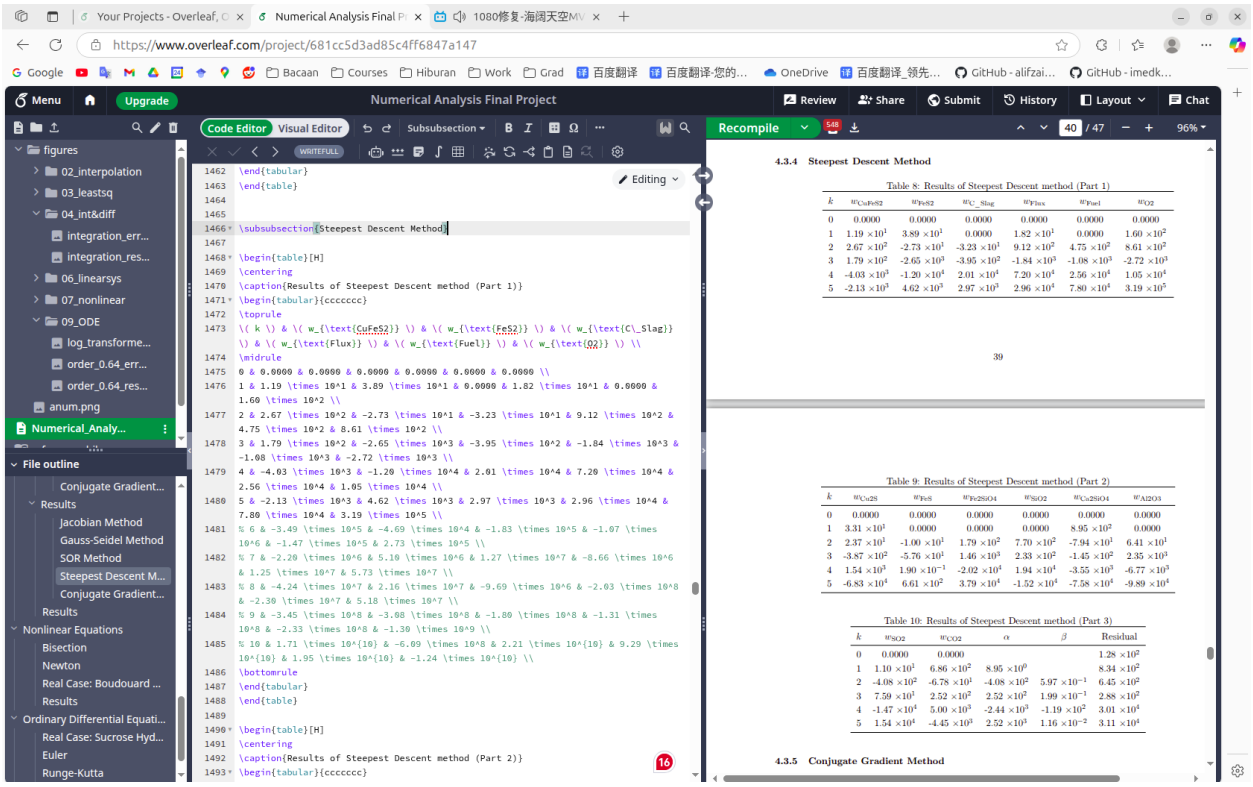


Figure 25: Only show half of max iteration :(

4.4.5 Conjugate Gradient Method

Table 18: Results of Conjugate Gradient method (Part 1)

k	w_{CuFeS2}	w_{FeS2}	$w_{\text{C\_Slag}}$	w_{Flux}	w_{Fuel}	w_{O2}	w_{N2}
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	11.8534	38.8883	0.0000	18.2230	0.0000	160.1691	37.0633
2	26.4679	-31.0606	-4.2131	106.0731	62.0286	-0.8353	170.2829
3	39.1477	16.3453	-2.1001	148.9784	77.9697	156.0524	198.8193
4	-214.4401	-7050.3375	-1873.1774	-9624.0332	-4274.7193	-14682.9149	4999.7204
5	363.5734	7269.9871	1848.1179	10119.7885	4540.7178	15419.3319	-4452.4879
6	95.7469	-157.5146	-116.9182	-150.8443	-33.9928	-175.9652	587.9656
7	130.9044	63.2694	-93.9381	120.4240	93.1006	237.1970	557.1989
8	311.5840	1977.9058	165.9106	2580.0815	1194.4393	3198.6350	8.6722
9	-179.4649	-4390.7281	-797.0186	-5750.2975	-2519.0523	-6619.1756	2130.9367
10	342.5440	1710.9291	78.3454	2158.3552	1012.5862	2784.3617	236.2954

Table 19: Results of Conjugate Gradient method (Part 2)

k	w_{Cu2S}	w_{FeS}	w_{Fe2SiO4}	w_{SiO2}	w_{Ca2SiO4}	w_{Al2O3}	w_{Cu2O}
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	33.1360	0.0000	0.0000	0.0000	8.95 $\times 10^{2}$	0.0000	8.95 $\times 10^{1}$
2	-20.3315	-1.3067	2.34 $\times 10^{1}$	-5.32 $\times 10^{2}$	-1.04 $\times 10^{1}$	-5.49 $\times 10^{1}$	-6.78 $\times 10^{1}$
3	8.1490	-1.0944	1.58 $\times 10^{2}$	1.58 $\times 10^{2}$	-1.34 $\times 10^{1}$	1.59 $\times 10^{1}$	-1.42 $\times 10^{1}$
4	-2436.7036	-118.6226	-2.14 $\times 10^{3}$	-7.05 $\times 10^{3}$	-1.87 $\times 10^{3}$	-9.62 $\times 10^{3}$	-4.27 $\times 10^{3}$
5	2519.1301	116.9826	3.64 $\times 10^{2}$	7.27 $\times 10^{3}$	1.85 $\times 10^{3}$	1.01 $\times 10^{4}$	4.54 $\times 10^{3}$
6	-50.6906	-6.4989	9.57 $\times 10^{1}$	-1.58 $\times 10^{2}$	-1.17 $\times 10^{2}$	-1.51 $\times 10^{2}$	-3.40 $\times 10^{1}$
7	32.0940	-3.7953	1.31 $\times 10^{2}$	6.33 $\times 10^{1}$	-9.39 $\times 10^{1}$	1.20 $\times 10^{2}$	9.31 $\times 10^{1}$
8	823.9719	26.8669	3.12 $\times 10^{2}$	1.98 $\times 10^{3}$	1.66 $\times 10^{2}$	2.58 $\times 10^{3}$	1.19 $\times 10^{3}$
9	-1817.3784	-80.2385	-1.79 $\times 10^{2}$	-4.39 $\times 10^{3}$	-7.97 $\times 10^{2}$	-5.75 $\times 10^{3}$	-2.52 $\times 10^{3}$
10	712.1424	20.0331	3.43 $\times 10^{2}$	1.71 $\times 10^{3}$	7.83 $\times 10^{1}$	2.16 $\times 10^{3}$	1.01 $\times 10^{3}$

Table 20: Results of Conjugate Gradient method (Part 3)

k	w_{SO2}	w_{CO2}	α	β	Residual
0	0.0000	0.0000			127.8830
1	1.10 $\times 10^{1}$	6.86 $\times 10^{2}$	8.95 $\times 10^{0}$		834.2690
2	-4.08 $\times 10^{2}$	-6.78 $\times 10^{1}$	-4.08 $\times 10^{2}$	0.5970	644.5874
3	7.59 $\times 10^{1}$	0.2580	0.2580	0.1991	287.5950
4	-1.47 $\times 10^{4}$	5.00 $\times 10^{3}$	-2.44 $\times 10^{3}$	-1.19 $\times 10^{2}$	30098.1827
5	1.54 $\times 10^{4}$	-4.45 $\times 10^{3}$	2.52 $\times 10^{3}$	0.0116	31142.3866
6	-1.76 $\times 10^{2}$	5.88 $\times 10^{2}$	-5.07 $\times 10^{1}$	-0.0056	801.7977
7	5.57 $\times 10^{2}$	3.21 $\times 10^{1}$	3.21 $\times 10^{1}$	0.2083	717.6400
8	8.67 $\times 10^{0}$	1.83 $\times 10^{1}$	1.83 $\times 10^{1}$	1.82 $\times 10^{1}$	6810.7401
9	2.13 $\times 10^{3}$	-1.82 $\times 10^{3}$	-1.82 $\times 10^{3}$	-0.0672	14524.4245
10	2.36 $\times 10^{2}$	0.0142	0.0142	0.1699	5987.2638

4.5 Comparison

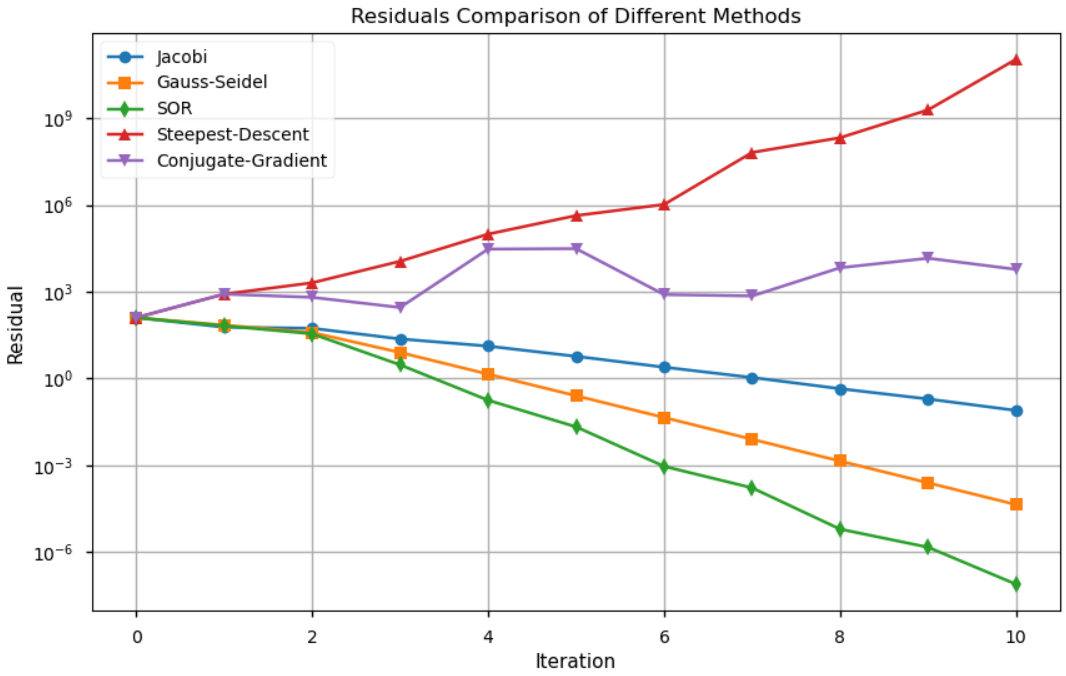


Figure 26: Residual comparison from different method

5 Nonlinear Equations

5.1 Real Case: Boudouard Reaction Equilibrium

The Boudouard reaction is a chemical equilibrium reaction that describes the conversion of carbon monoxide (CO) to carbon dioxide (CO_2) and solid carbon (C) at high temperatures. The reaction is represented as:

$$2\text{CO} \leftrightarrow \text{CO}_2 + \text{C} \tag{74}$$

This reaction is important in various industrial processes, such as the production of synthesis gas and the reduction of iron ore.

Given the fraction of CO (x_{CO}) in the gas mixture, the equilibrium constant K for the Boudouard reaction can be expressed as:

$$K = \frac{P_{\text{CO}_2} \cdot P_{\text{C}}}{P_{\text{CO}}^2} \tag{75}$$

Where:

- P_{CO} is the partial pressure of CO.
- P_{CO_2} is the partial pressure of CO_2.
- P_{C} is the partial pressure of solid carbon (which is often considered to be 1 atm).

Given $x_{\text{CO}} = \frac{n_{\text{CO}}}{n_{\text{CO}} + n_{\text{CO}_2}}$, we can express the partial pressures in terms of x_{CO}:

$$P_{\text{CO}} = x_{\text{CO}} \cdot P_{\text{total}} \tag{76}$$

$$P_{\text{CO}_2} = (1 - x_{\text{CO}}) \cdot P_{\text{total}} \tag{77}$$

Assuming $P_{\text{total}} = 1$ atm for simplicity, the equilibrium constant K becomes:

$$K = \frac{(1 - x_{\text{CO}})}{x_{\text{CO}}^2} \tag{78}$$

Taking the natural logarithm of both sides:

$$\ln K = \ln \left(\frac{1 - x_{\text{CO}}}{x_{\text{CO}}^2} \right) \tag{79}$$

The Gibbs free energy change (ΔG) for the reaction can be related to the equilibrium constant K by:

$$\Delta G = -RT \ln K \tag{80}$$

Where:

- R is the universal gas constant.
- T is the temperature in Kelvin.

The enthalpy change (ΔH) and entropy change (ΔS) for the reaction can be calculated using the Shomate equation parameters. The function $f(T)$ representing the equilibrium condition is:

$$f(T) = \ln K + \frac{\Delta H(T)}{RT} - \frac{\Delta S(T)}{R} \tag{81}$$

The Shomate parameters for CO, CO_2, and $C_(s)$ are given as follows:

$$\begin{aligned}
&\text{CO:} \quad A_1 = 25.56759, \quad B_1 = 6.096130, \quad C_1 = 4.054656, \quad D_1 = -2.671301, \quad E_1 = 0.131021 \\
&\text{CO}_2\text{:} \quad A_2 = 24.99735, \quad B_2 = 55.18696, \quad C_2 = -33.69137, \quad D_2 = 7.948387, \quad E_2 = -0.136638 \\
&\text{C(s):} \quad A_3 = 17.7289, \quad B_3 = 28.0988, \quad C_3 = -4.21434, \quad D_3 = 0.218050, \quad E_3 = -0.000281
\end{aligned} \tag{82}$$

The Δ parameters for the reaction $2CO \rightarrow CO_2 + C$ are calculated as:

$$\begin{aligned}
\Delta A &= A_2 + A_3 - 2A_1 \\
\Delta B &= B_2 + B_3 - 2B_1 \\
\Delta C &= C_2 + C_3 - 2C_1 \\
\Delta D &= D_2 + D_3 - 2D_1 \\
\Delta E &= E_2 + E_3 - 2E_1
\end{aligned} \tag{83}$$

The enthalpy change (ΔH) and entropy change (ΔS) as functions of temperature are given by:

$$\begin{aligned}
\Delta H(T) = \Delta H_{298} + \Delta A(T - 298) + \frac{\Delta B}{1000}\left(\frac{T^2}{2} - \frac{298^2}{2}\right) + \frac{\Delta C}{10^6}\left(\frac{T^3}{3} - \frac{298^3}{3}\right) \\
+ \frac{\Delta D}{10^9}\left(\frac{T^4}{4} - \frac{298^4}{4}\right) + \Delta E \times 10^6\left(-\frac{1}{T} + \frac{1}{298}\right)
\end{aligned} \tag{84}$$

$$\begin{aligned}
\Delta S(T) = \Delta S_{298} + \Delta A \ln\left(\frac{T}{298}\right) + \frac{\Delta B}{1000}(T - 298) + \frac{\Delta C}{2 \times 10^6}(T^2 - 298^2) \\
+ \frac{\Delta D}{3 \times 10^9}(T^3 - 298^3) + \Delta E \times 10^6\left(-\frac{1}{2T^2} + \frac{1}{2 \times 298^2}\right)
\end{aligned} \tag{85}$$

Where:

- $\Delta H_{298} = -172459$ J/mol
- $\Delta S_{298} = -175.79$ J/(mol‘ůK)
- $R = 8.314$ J/(mol‘ůK)

5.2 Method

5.2.1 Bisection

The Bisection method is a root-finding method that repeatedly bisects an interval and then selects a subinterval in which a root must lie for further processing. The algorithm is as follows:

Algorithm 20 Bisection Method

Require: Function f, interval $[a, b]$, maximum iterations max_iter
Ensure: Approximation of the root of $f(x) = 0$
0: Ensure $f(a) \cdot f(b) < 0$ (i.e., f changes sign over $[a, b]$)
0: Initialize error $\leftarrow b - a$
0: **for** $n = 1$ to max_iter **do**
0: Compute the midpoint $c \leftarrow \frac{a+b}{2}$
0: Evaluate $f(c)$
0: Update the error error $\leftarrow b - a$
0: **if** $f(a) \cdot f(c) < 0$ **then**
0: $b \leftarrow c$
0: **else**
0: $a \leftarrow c$
0: **end if**
0: **end for**
0: **return** c as the best approximation $=0$

Python snippet for the bisection method:

```
def bisection(x_CO, T_low=600, T_high=1200, max_iter=100):
    iterations = []
    for n in range(max_iter):
        T_mid = (T_low + T_high) / 2
        F_mid = f(T_mid, x_CO)
        F_low = f(T_low, x_CO)
        error = T_high - T_low
        iterations.append([n, T_mid, F_mid, error])
        if F_mid * F_low < 0:
            T_high = T_mid
        else:
            T_low = T_mid
    return pd.DataFrame(iterations, columns=["Iteration", "T", "f(T)", "Error"])
```

5.2.2 Newton

The Newton-Raphson method is an iterative root-finding algorithm that uses the first derivative of the function to approximate the root. The algorithm is as follows:

Algorithm 21 Newton Method

Require: Function f, initial guess x_0, maximum iterations max_iter
Ensure: Approximation of the root of $f(x) = 0$
0: Initialize $x \leftarrow x_0$
0: **for** $n = 1$ to max_iter **do**
0: Compute $f(x)$ and its derivative $f'(x)$
0: Update the guess $x_{\text{new}} \leftarrow x - \frac{f(x)}{f'(x)}$
0: Compute the error error $\leftarrow |x_{\text{new}} - x|$
0: Update $x \leftarrow x_{\text{new}}$
0: **end for**
0: **return** x as the best approximation =0

Python snippet for the newton method:

```
def newton_raphson(x_CO, T_guess=800, tol=1e-6, max_iter=100):
    T = T_guess
    iterations = []
    for n in range(max_iter):
        F = f(T, x_CO)
        dT = 1e-3
        F_plus = f(T + dT, x_CO)
        dFdT = (F_plus - F) / dT
        T_new = T - F / dFdT
        error = abs(T_new - T)
        iterations.append([n, T, F, error])
        # if error < tol:
        #     break
        T = T_new
    return pd.DataFrame(iterations, columns=["Iteration", "T", "f(T)", "Error"])
```

5.3 Python Snippet for various method

```
\begin{lstlisting}[style=custompython]
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import os

# Shomate parameters (CO, CO‘‘ĆĆ, C(s))
A1, B1, C1, D1, E1 = 25.56759, 6.096130, 4.054656, -2.671301, 0.131021     # CO
A2, B2, C2, D2, E2 = 24.99735, 55.18696, -33.69137, 7.948387, -0.136638    # CO‘‘ĆĆ
A3, B3, C3, D3, E3 = 17.7289, 28.0988, -4.21434, 0.218050, -0.000281       # C(s)

# ‘Ť parameters for 2CO ‘‘ĘŠ CO‘‘ĆĆ + C
delta_A = A2 + A3 - 2*A1
delta_B = B2 + B3 - 2*B1
delta_C = C2 + C3 - 2*C1
delta_D = D2 + D3 - 2*D1
```

```
delta_E = E2 + E3 - 2*E1

# Standard values
delta_H_298 = -172459  # J/mol
delta_S_298 = -175.79  # J/(mol‘ůK)
R = 8.314

# Functions for enthalpy and entropy changes
def delta_H(T):
    term1 = delta_A * (T - 298)
    term2 = (delta_B / 1000) * (T**2 / 2 - 298**2 / 2)
    term3 = (delta_C / 1e6) * (T**3 / 3 - 298**3 / 3)
    term4 = (delta_D / 1e9) * (T**4 / 4 - 298**4 / 4)
    term5 = delta_E * 1e6 * (-1/T + 1/298)
    return delta_H_298 + term1 + term2 + term3 + term4 + term5

def delta_S(T):
    term1 = delta_A * np.log(T / 298)
    term2 = (delta_B / 1000) * (T - 298)
    term3 = (delta_C / 2e6) * (T**2 - 298**2)
    term4 = (delta_D / 3e9) * (T**3 - 298**3)
    term5 = delta_E * 1e6 * (-1/(2*T**2) + 1/(2*298**2))
    return delta_S_298 + term1 + term2 + term3 + term4 + term5

# Equilibrium function
def f(T, x_CO):
    K = (1 - x_CO) / (x_CO**2)
    lnK = np.log(K)
    dH = delta_H(T)
    dS = delta_S(T)
    return lnK + dH/(R*T) - dS/R

# Newton-Raphson Solver
def newton_raphson(x_CO, T_guess=800, tol=1e-6, max_iter=100):
    T = T_guess
    iterations = []
    for n in range(max_iter):
        F = f(T, x_CO)
        dT = 1e-3
        F_plus = f(T + dT, x_CO)
        dFdT = (F_plus - F) / dT
        T_new = T - F / dFdT
        error = abs(T_new - T)
        iterations.append([n, T, F, error])
        T = T_new
    return pd.DataFrame(iterations, columns=["Iteration", "T", "f(T)", "Error"])

```

```python
# Bisection Solver
def bisection(x_CO, T_low=600, T_high=1200, max_iter=100):
    iterations = []
    for n in range(max_iter):
        T_mid = (T_low + T_high) / 2
        F_mid = f(T_mid, x_CO)
        F_low = f(T_low, x_CO)
        error = T_high - T_low
        iterations.append([n, T_mid, F_mid, error])
        if F_mid * F_low < 0:
            T_high = T_mid
        else:
            T_low = T_mid
    return pd.DataFrame(iterations, columns=["Iteration", "T", "f(T)", "Error"])

# Solve for different x_CO values
x_CO_values = [0.1, 0.3, 0.5, 0.7, 0.9]
results_dir = "07_nonlinear/results"
os.makedirs(results_dir, exist_ok=True)

# Generate and save results
for x_CO in x_CO_values:
    df_nr = newton_raphson(x_CO, max_iter=20)
    df_bs = bisection(x_CO, max_iter=20)
    with pd.ExcelWriter(f"{results_dir}/xCO_{x_CO:.1f}_results.xlsx") as writer:
        df_nr.to_excel(writer, sheet_name="Newton-Raphson", index=False)
        df_bs.to_excel(writer, sheet_name="Bisection", index=False)

# Plot x_CO vs. T
plt.figure(figsize=(8, 5))
x_plot = x_CO_values
T_plot_nr = [newton_raphson(x, max_iter=20).iloc[-1]["T"] for x in x_plot]
plt.plot(x_plot, T_plot_nr, 'r-', marker='o', label="Newton")
plt.xlabel(r"$x_{\mathrm{CO}}$ = CO/(CO+CO‘‘ĆĆ)")
plt.ylabel("Temperature (K)")
plt.title("Boudouard Reaction Equilibrium")
plt.grid(True)
plt.savefig(f"{results_dir}/xCO_vs_T.png")
plt.close()

# Plot error convergence for Newton-Raphson
plt.figure(figsize=(10, 6))
markerss = ['o', 's', 'd', '^', 'v', 'p', '*', 'h', '+', 'x']
for i, x_CO in enumerate(x_CO_values):
    df = pd.read_excel(f"{results_dir}/xCO_{x_CO:.1f}_results.xlsx", sheet_name="
        Newton-Raphson")
```

```
    plt.semilogy(df["Iteration"], df["Error"], marker=markerss[i], label=f"$x_{{\\mathrm{{CO}}}}$ = {x_CO}")
plt.xlabel("Iteration")
plt.ylabel("Error (log scale)")
plt.title("Newton Error Convergence")
plt.grid(True, which="both", ls="--")
plt.legend()
plt.tight_layout()
plt.savefig(f"{results_dir}/newton_error_convergence.png")
plt.close()

# Plot error convergence for Bisection
plt.figure(figsize=(10, 6))
for i, x_CO in enumerate(x_CO_values):
    df = pd.read_excel(f"{results_dir}/xCO_{x_CO:.1f}_results.xlsx", sheet_name="Bisection")
    plt.semilogy(df["Iteration"], df["Error"], marker=markerss[i], label=f"$x_{{\\mathrm{{CO}}}}$ = {x_CO}")
plt.xlabel("Iteration")
plt.ylabel("Error (log scale)")
plt.title("Bisection Error Convergence")
plt.grid(True, which="both", ls="--")
plt.legend()
plt.tight_layout()
plt.savefig(f"{results_dir}/bisection_error_convergence.png")
plt.close()

# Plot value convergence for Newton-Raphson
plt.figure(figsize=(10, 6))
for i, x_CO in enumerate(x_CO_values):
    df = pd.read_excel(f"{results_dir}/xCO_{x_CO:.1f}_results.xlsx", sheet_name="Newton-Raphson")
    plt.plot(df["Iteration"], df["T"], marker=markerss[i], label=f"T at $x_{{\\mathrm{{CO}}}}$ = {x_CO}")
plt.xlabel("Iteration")
plt.ylabel("T (K)")
plt.title("Newton Temperature Convergence")
plt.grid(True, which="both", ls="--")
plt.legend()
plt.tight_layout()
plt.savefig(f"{results_dir}/Newton_Temperature_convergence.png")
plt.close()

# Plot value convergence for Bisection
plt.figure(figsize=(10, 6))
for i, x_CO in enumerate(x_CO_values):
```

```
    df = pd.read_excel(f"{results_dir}/xCO_{x_CO:.1f}_results.xlsx", sheet_name="Bisection")
    plt.plot(df["Iteration"], df["T"], marker=markerss[i], label=f"T at $x_{{\\mathrm{{CO}}}}$ = {x_CO}")
plt.xlabel("Iteration")
plt.ylabel("T (K)")
plt.title("Bisection Temperature Convergence")
plt.grid(True, which="both", ls="--")
plt.legend()
plt.tight_layout()
plt.savefig(f"{results_dir}/Bisection_Temperature_convergence.png")
plt.close()
```

5.4 Results

5.4.1 Bisection

Table 21: Bisection Method Results for Different x_{CO} Values

Iteration	$x_{CO} = 0.3$			$x_{CO} = 0.5$			$x_{CO} = 0.7$		
	T	$f(T)$	Error	T	$f(T)$	Error	T	$f(T)$	Error
0	900	-0.54	600	900	-1.90	600	900	-3.09	600
1	1050	2.50	300	1050	1.14	300	1050	-0.04	300
2	975	1.10	150	975	-0.25	150	1125	1.15	150
3	937.50	0.32	75	1012.50	0.47	75	1087.50	0.57	75
4	918.75	-0.11	37.50	993.75	0.12	37.50	1068.75	0.27	37.50
5	928.13	0.11	18.75	984.38	-0.07	18.75	1059.38	0.11	18.75
6	923.44	0.00	9.38	989.06	0.02	9.38	1054.69	0.04	9.38
7	921.09	-0.05	4.69	986.72	-0.02	4.69	1052.34	0.00	4.69
8	922.27	-0.02	2.34	987.89	0.00	2.34	1053.52	0.02	2.34
9	922.85	-0.01	1.17	987.30	-0.01	1.17	1052.93	0.01	1.17
10	923.14	0.00	0.59	987.60	0.00	0.59	1052.64	0.00	0.59
11	923.29	0.00	0.29	987.74	0.00	0.29	1052.49	0.00	0.29
12	923.36	0.00	0.15	987.82	0.00	0.15	1052.56	0.00	0.15
13	923.33	0.00	0.07	987.78	0.00	0.07	1052.60	0.00	0.07
14	923.35	0.00	0.04	987.80	0.00	0.04	1052.62	0.00	0.04
15	923.36	0.00	0.02	987.81	0.00	0.02	1052.61	0.00	0.02
16	923.36	0.00	0.01	987.80	0.00	0.01	1052.61	0.00	0.01
17	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
18	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
19	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
20	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00

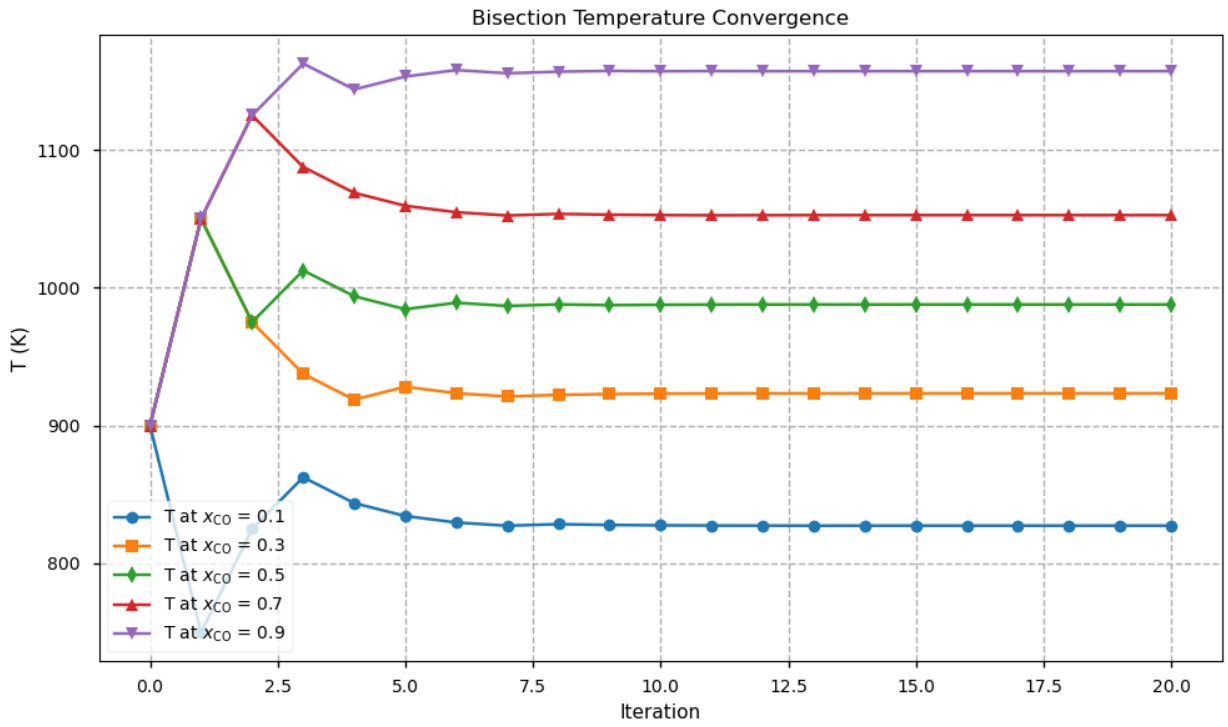


Figure 27: Temperature convergence using bisection method

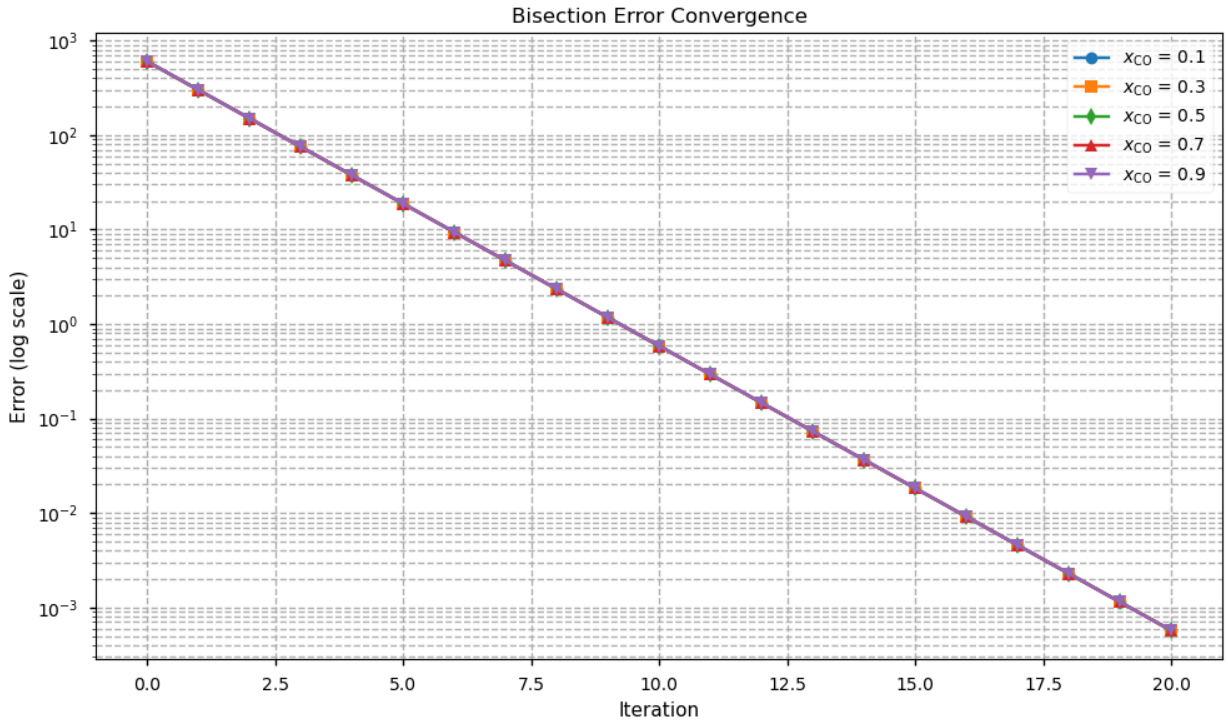


Figure 28: Error from bisection method

5.4.2 Newton

Table 22: Newton Method Results for Different x_{CO} Values

Iteration	$x_{CO} = 0.3$			$x_{CO} = 0.5$			$x_{CO} = 0.7$		
	T	$f(T)$	Error	T	$f(T)$	Error	T	$f(T)$	Error
0	800	-3.26	105.87	800	-4.62	149.93	800	-5.81	188.34
1	905.87	-0.40	17.13	949.93	-0.77	36.29	988.34	-1.17	59.99
2	923.00	-0.01	0.36	986.23	-0.03	1.57	1048.33	-0.07	4.26
3	923.36	0.00	0.00	987.80	0.00	0.00	1052.59	0.00	0.02
4	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
5	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
6	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
7	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
8	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
9	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
10	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
11	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
12	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
13	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
14	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
15	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
16	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
17	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
18	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
19	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00
20	923.36	0.00	0.00	987.80	0.00	0.00	1052.61	0.00	0.00

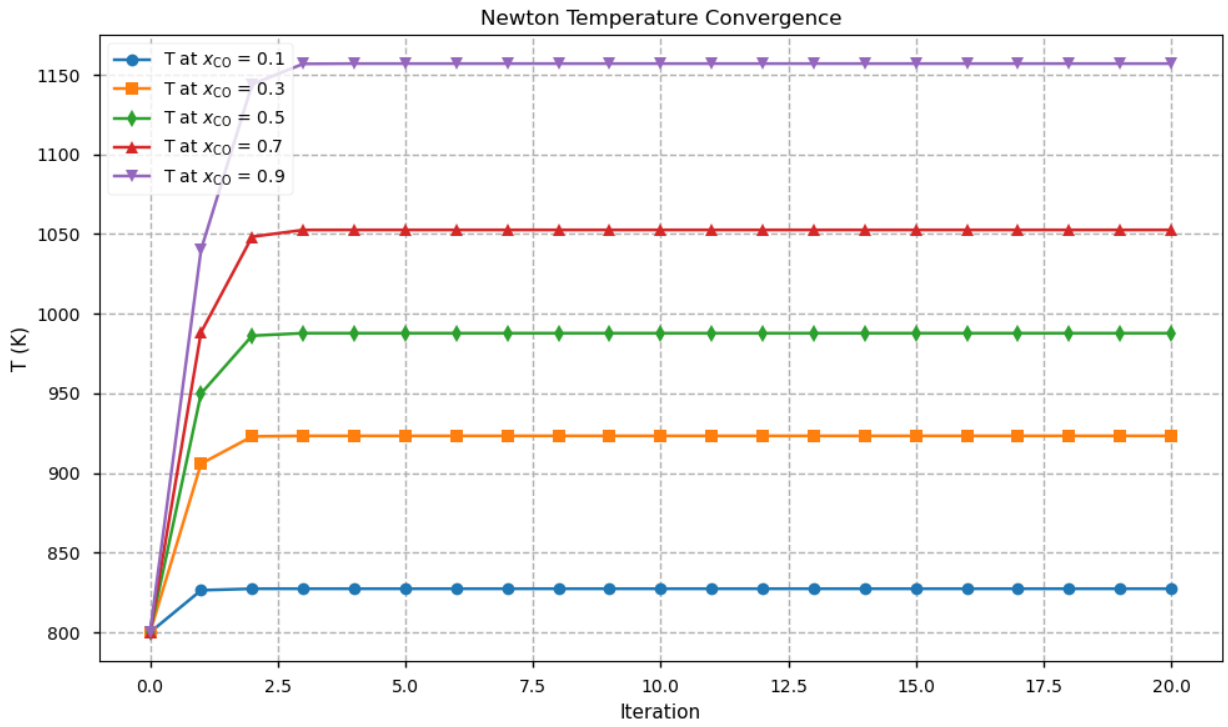


Figure 29: Temperature convergence using newton method

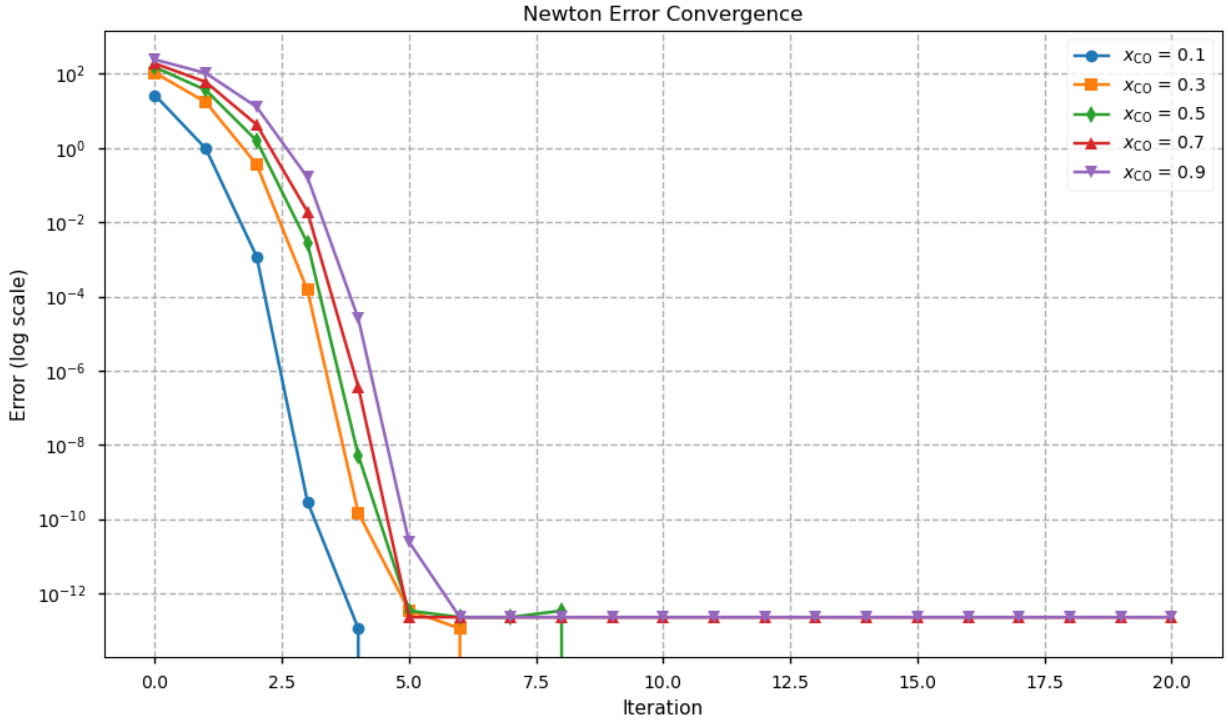


Figure 30: Error from newton method

5.4.3 Boudouard Reaction

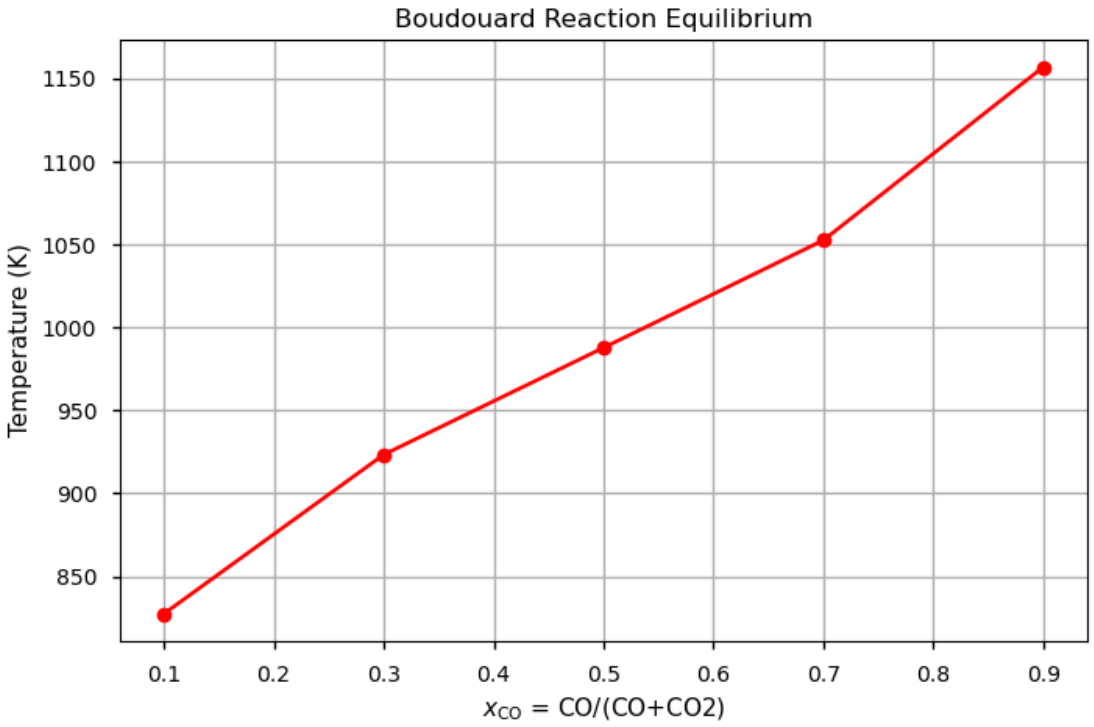


Figure 31: Boudouard Reaction from known CO fraction

5.4.4 Key Observations

- The Bisection method is guaranteed to converge if the function changes sign over the interval. It is robust but can be slow.
- The Newton-Raphson method converges quickly if the initial guess is close to the root. However, it requires the derivative of the function and may not converge if the initial guess is not good.

6 Ordinary Differential Equation

6.1 Real Case: Sucrose Hydrolysis Reaction Profile

Reaction kinetics is the study of the rates of chemical reactions and the factors that influence these rates. For sucrose hydrolysis, the reaction rate is described by the rate equation above. The reaction order n indicates how the rate of reaction changes with the concentration of sucrose. For example:

- If $n = 1$, the reaction is first-order, meaning the rate is directly proportional to the concentration of sucrose.
- If $n = 2$, the reaction is second-order, meaning the rate is proportional to the square of the concentration.

The reaction rate constant k is a proportionality constant that depends on factors such as temperature and the presence of a catalyst. It quantifies how quickly the reaction proceeds under given conditions.

Sucrose hydrolysis is an acid-catalyzed reaction governed by the rate equation:

$$-\frac{dC_A}{dt} = k{C_A}^n \tag{86}$$

where:

- C_A: Concentration of sucrose (reactant)
- k: Reaction rate constant (depends on temperature and catalyst)
- n: Reaction order (determines rate dependence on concentration)

The code calculates n and k using experimental data and logarithmic transformation:

$$\ln(-\frac{dC_A}{dt}) = \ln(k) + n\ln(C_A) \tag{87}$$

- Numerical derivatives approximate $\frac{dC_A}{dt}$
- Least squares regression determines n (slope) and $k = e^{\text{intercept}}$

Table 23: Experimental Data for Sucrose Hydrolysis

t (hours)	C_A (millimol/liter)
0	1.00
1	0.84
2	0.68
3	0.53
4	0.38
5	0.27
6	0.16
7	0.09
8	0.04
9	0.018
10	0.006
11	0.0025

6.2 Method

6.2.1 Euler

Algorithm 22 Euler Method

Require: Initial time t_0, initial concentration C_{A0}, step size h, final time t_f, ODE function $f(t, C_A)$
Ensure: Approximate concentration profile
0: Initialize $C_A(t_0) = C_{A0}$
0: **for** $t = t_0 + h$ to t_f step h **do**
0: $C_A(t) = C_A(t-h) + h \cdot f(t-h, C_A(t-h))$
0: **end for**=0

Python snippet for the Euler method:

```
def euler(self) -> Tuple[np.ndarray, np.ndarray]:
        y = np.zeros(len(self.t))
        y[0] = self.y0
        for i in range(1, len(self.t)):
            y[i] = y[i-1] + self.h * self.f(self.t[i-1], y[i-1])

        return self.t, y
```

Key features:

- First-order accuracy
- Simplest numerical integration method
- Prone to instability for stiff equations

6.2.2 Runge-Kutta

Algorithm 23 4th Order Runge-Kutta Method

Require: Same inputs as Euler method
Ensure: More accurate concentration profile
0: **for** $t = t_0 + h$ to t_f step h **do**
0: $k_1 = f(t - h, C_A(t - h))$
0: $k_2 = f(t - \frac{h}{2}, C_A(t - h) + \frac{h}{2}k_1)$
0: $k_3 = f(t - \frac{h}{2}, C_A(t - h) + \frac{h}{2}k_2)$
0: $k_4 = f(t, C_A(t - h) + hk_3)$
0: $C_A(t) = C_A(t - h) + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$
0: **end for**=0

Python snippet for the Runge-Kutte 4 method:

```
def runge_kutta4(self) -> Tuple[np.ndarray, np.ndarray]:
    y = np.zeros(len(self.t))
    y[0] = self.y0
    for i in range(1, len(self.t)):
        t_prev = self.t[i-1]
        y_prev = y[i-1]
        h = self.h
        k1 = self.f(t_prev, y_prev)
        k2 = self.f(t_prev + h/2, y_prev + h/2 * k1)
        k3 = self.f(t_prev + h/2, y_prev + h/2 * k2)
        k4 = self.f(t_prev + h, y_prev + h * k3)
        y[i] = y_prev + h/6 * (k1 + 2*k2 + 2*k3 + k4)

    return self.t, y
```

Key features:

- Fourth-order accuracy
- Balances computational effort and precision
- Requires four function evaluations per step

6.3 Python snippet for various method

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import os
from typing import Callable, Optional, Tuple

# Define ODE solver class
class ODESolver:
    def __init__(self,
                 f: Callable[[float, float], float],
```

```
                  y0: float,
                  t0: float,
                  tf: float,
                  h: float,
                  primitive: Optional[Callable[[float], float]] = None):

        self.f = f
        self.y0 = y0
        self.t0 = t0
        self.tf = tf
        self.h = h
        self.primitive = primitive

        # Create time array
        self.t = np.arange(t0, tf + h, h)

    def euler(self) -> Tuple[np.ndarray, np.ndarray]:
        y = np.zeros(len(self.t))
        y[0] = self.y0

        for i in range(1, len(self.t)):
            y[i] = y[i-1] + self.h * self.f(self.t[i-1], y[i-1])

        return self.t, y

    def runge_kutta4(self) -> Tuple[np.ndarray, np.ndarray]:
        y = np.zeros(len(self.t))
        y[0] = self.y0

        for i in range(1, len(self.t)):
            t_prev = self.t[i-1]
            y_prev = y[i-1]
            h = self.h

            k1 = self.f(t_prev, y_prev)
            k2 = self.f(t_prev + h/2, y_prev + h/2 * k1)
            k3 = self.f(t_prev + h/2, y_prev + h/2 * k2)
            k4 = self.f(t_prev + h, y_prev + h * k3)

            y[i] = y_prev + h/6 * (k1 + 2*k2 + 2*k3 + k4)

        return self.t, y

# Experimental data
t_exp = np.array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11])
CA_exp = np.array([1.0, 0.84, 0.68, 0.53, 0.38, 0.27, 0.16, 0.09, 0.04, 0.018,
    0.006, 0.0025])
```

```

# Function to define the ODE for different reaction orders
def create_f(n: float, k: float) -> Callable[[float, float], float]:
    def f(t: float, CA: float) -> float:
        return -k * CA**n
    return f

# Least squares fit function
def least_squares_fit(x, y, n):
    G = np.zeros((n+1, n+1))
    b = np.zeros(n+1)
    for j in range(n+1):
        for k in range(n+1):
            G[j, k] = np.sum(x**(j + k))
        b[j] = np.sum(y * x**j)
    try:
        beta = np.linalg.solve(G, b)
    except np.linalg.LinAlgError:
        beta = np.linalg.pinv(G) @ b  # Fallback to pseudo-inverse
    return beta, G, b

# Calculate the derivative using finite differences
dCA_dt = np.zeros_like(CA_exp)
for i in range(1, len(CA_exp) - 1):
    dCA_dt[i] = (CA_exp[i+1] - CA_exp[i-1]) / (t_exp[i+1] - t_exp[i-1])
dCA_dt[0] = (CA_exp[1] - CA_exp[0]) / (t_exp[1] - t_exp[0])
dCA_dt[-1] = (CA_exp[-1] - CA_exp[-2]) / (t_exp[-1] - t_exp[-2])

# Avoid log of negative or zero values
valid_indices = CA_exp > 0
ln_CA = np.log(CA_exp[valid_indices])
ln_dCA_dt = np.log(-dCA_dt[valid_indices])

# Perform least squares fit for the linear equation ln(-dCA/dt) = ln(k) + n*ln(CA)
beta, G, b = least_squares_fit(ln_CA, ln_dCA_dt, 1)
n_estimate = beta[1]
k_estimate = np.exp(beta[0])

# Create directory for least squares data if it doesn't exist
os.makedirs('09_ODE/least_square_data', exist_ok=True)

# Save Gram matrix, right-hand side vector, and least squares results to Excel
with pd.ExcelWriter('09_ODE/least_square_data/least_squares_results.xlsx') as
    writer:
    pd.DataFrame({'ln_CA': ln_CA, 'ln_dCA_dt': ln_dCA_dt}).to_excel(writer,
        sheet_name='Data', index=False)
```

```
    pd.DataFrame(G, columns=[f'G_{i}' for i in range(G.shape[1])]).to_excel(writer, sheet_name='Gram_Matrix', index=False)
    pd.DataFrame({'b': b}).to_excel(writer, sheet_name='RHS_Vector', index=False)
    pd.DataFrame({'beta': beta}).to_excel(writer, sheet_name='Results', index=False)

# Plot the log-transformed data
plt.figure(figsize=(10, 6))
plt.style.use('seaborn-v0_8-notebook')
plt.scatter(ln_CA, ln_dCA_dt, facecolors='none', edgecolors='black', linewidths=1, label='Experimental Data')
plt.plot(ln_CA, beta[0] + beta[1] * ln_CA, 'r-', label='Least Squares Fit')
plt.xlabel(r'$\ln(C_A)$')
plt.ylabel(r'$\ln(-dC_A/dt)$')
plt.title('Log-Transformed Rate Data')
plt.legend()
plt.grid(True)

# Create directory for plots if it doesn't exist
os.makedirs('09_ODE/plots', exist_ok=True)
plt.savefig('09_ODE/plots/log_transformed_rate_data.png')
plt.close()

# Function to find the best reaction order and constant
def find_best_order_and_constant():
    orders = [0.5, n_estimate, 0.7, 1.1]
    k_guess = k_estimate

    for n in orders:
        f = create_f(n, k_guess)
        solver = ODESolver(f, y0=1.0, t0=0, tf=11, h=1)
        df = solver.solve_and_compare()
        df['Experimental'] = CA_exp

        if 'Euler' in df.columns:
            df['Euler Error'] = np.abs(df['Euler'] - df['Experimental'])
        if 'Runge-Kutta4' in df.columns:
            df['RK4 Error'] = np.abs(df['Runge-Kutta4'] - df['Experimental'])

        print(f"Results for reaction order {n:0,.2f}:")
        print(df[['t', 'Euler', 'Runge-Kutta4', 'Experimental', 'Euler Error', 'RK4 Error']])
        print("\n")

        # Create directory for results if it doesn't exist
        os.makedirs('09_ODE/results', exist_ok=True)
        df.to_excel(f'09_ODE/results/order_{n:0,.2f}_results.xlsx', index=False)
```

```
        # Plot results for this reaction order
        plt.figure(figsize=(10, 6))
        plt.style.use('seaborn-v0_8-notebook')
        plt.scatter(df['t'], df['Experimental'], facecolors='none', edgecolors='
            black', linewidths=1, label='Experimental')
        plt.plot(df['t'], df['Euler'], 'b-', marker='o', label='Euler')
        plt.plot(df['t'], df['Runge-Kutta4'], 'r-', marker='s', label='Runge-Kutta
             4')
        plt.xlabel('Time (hr)')
        plt.ylabel('Concentration (millimol/liter)')
        plt.title(f'Reaction Order {n:0,.2f}')
        plt.legend()
        plt.grid(True)
        plt.savefig(f'09_ODE/plots/order_{n:0,.2f}_results.png')
        plt.close()

# Run the analysis
find_best_order_and_constant()
```

6.4 Results

The estimated reaction order n and rate constant k are crucial for understanding the reaction mechanism and predicting the reaction profile. The results from the least squares regression provide the following estimates:

- Estimated reaction order $n \approx 0.64$
- Estimated rate constant $k \approx 0.22$

These values indicate that the reaction is slightly more than first-order, suggesting that the rate of hydrolysis increases slightly faster than linearly with the concentration of sucrose. The rate constant k provides a measure of the reaction's speed under the given conditions.

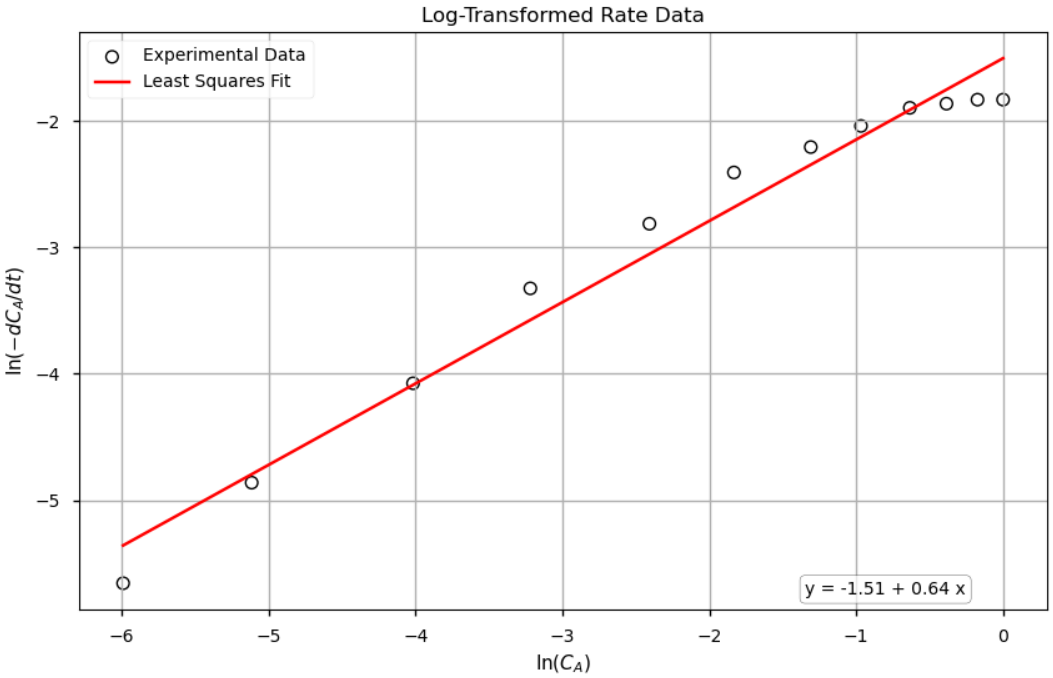


Figure 32: Interpolation data

The numerical solutions using Euler's method and the 4th order Runge-Kutta method were compared to the experimental data. The results are summarized in the following table:

Table 24: Comparison of Numerical Methods for Sucrose Hydrolysis

t	Euler	Runge-Kutta4	Experimental	Euler Error	RK4 Error
0	1.00	1.00	1.00	0.00	0.00
1	0.78	0.79	0.84	0.06	0.05
2	0.59	0.62	0.68	0.09	0.06
3	0.43	0.47	0.53	0.10	0.06
4	0.30	0.34	0.38	0.08	0.04
5	0.20	0.24	0.27	0.07	0.03
6	0.12	0.16	0.16	0.04	0.00
7	0.06	0.10	0.09	0.03	0.01
8	0.03	0.06	0.04	0.01	0.02
9	0.00	0.03	0.02	0.01	0.01
10	0.00	0.01	0.01	0.01	0.01
11		0.00	0.00		0.00

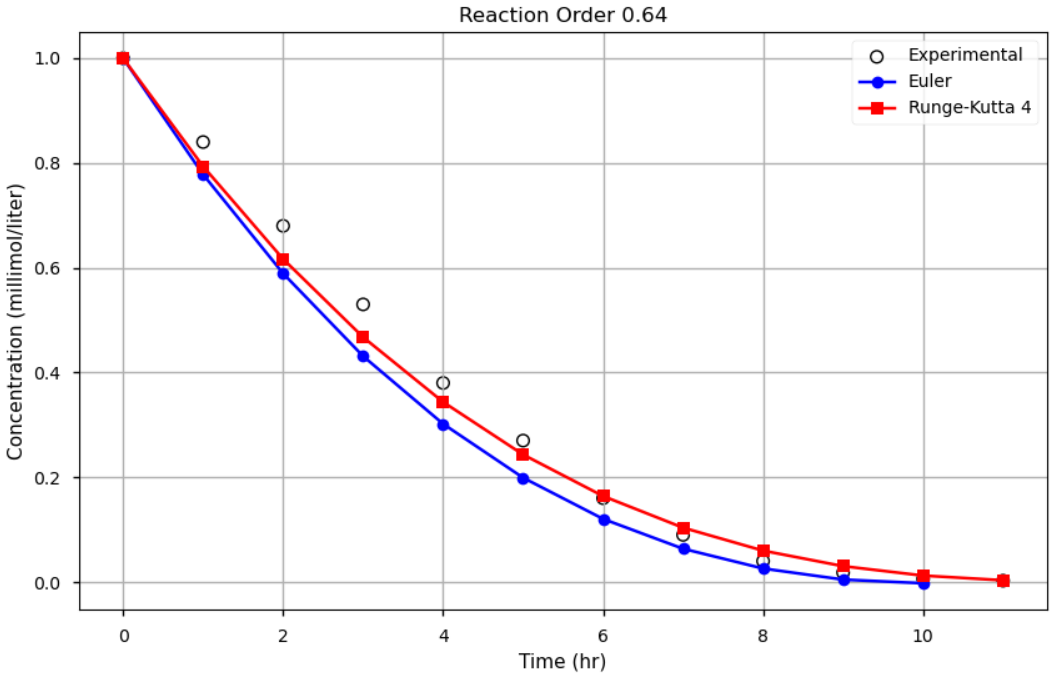


Figure 33: Reaction profile result

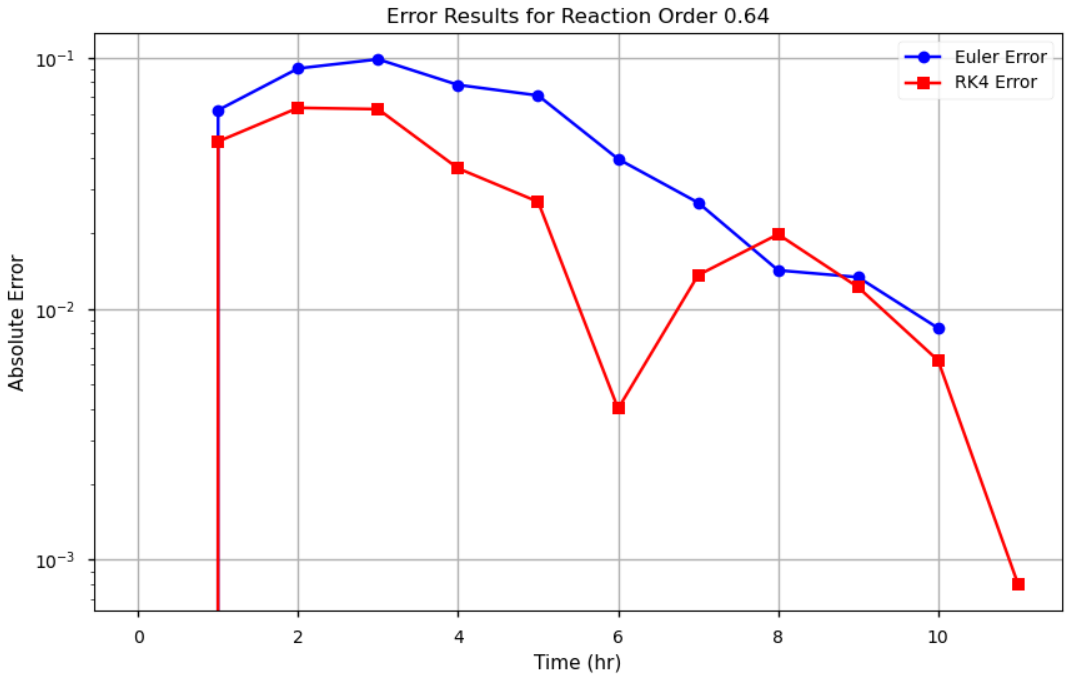


Figure 34: Error comparison

6.5 Key Observations

- The estimated reaction order (n) determines the rate equation's nonlinearity
- Runge-Kutta 4 demonstrates superior accuracy compared to Euler method
- Experimental validation shows best match at $n \approx 0.64$
- Error analysis highlights RK4's effectiveness in minimizing concentration prediction errors
- Numerical solutions must satisfy physical bounds (non-negative concentrations)