Dissertation

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Abstract

This thesis investigates the theory and applications of orthogonal polynomials in approximation theory, integrating foundational analysis with modern computational methods. Beginning with the formulation of orthogonality in weighted inner product spaces and the derivation of the three-term recurrence relation, the study examines classical families such as Legendre, Chebyshev, Hermite, and Laguerre polynomials and their roles in minimizing approximation error in L^2 and L^∞ norms. The convergence behavior of orthogonal series is analyzed through Jackson-type estimates, Lebesgue constants, and asymptotic decay of coefficients, highlighting the influence of function smoothness and phenomena such as Gibbs oscillations. Computational aspects, including FFT-based coefficient evaluation and Gaussian quadrature, are connected to spectral methods for differential equations, demonstrating exponential convergence for smooth solutions. The work further extends to non-classical weights and Sobolev orthogonal polynomials, emphasizing their relevance in variational formulations and energy norm approximations.

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Chapter 1

Foundations of Orthogonal Polynomials and Approximation Theory

1.1 Introduction

Approximation theory is an important area of applied mathematics concerned with representing complicated functions by simpler and more manageable expressions. In many real-world problems arising in science, engineering, and data analysis, obtaining exact analytical solutions is often difficult or even impossible. For this reason, approximation methods play a significant role in developing practical numerical solutions. Orthogonal polynomials are particularly valuable in approximation techniques because of their strong analytical properties, numerical stability, and ability to minimize approximation errors efficiently. They provide a solid mathematical framework for studying convergence behavior, error estimation, and efficient numerical computation. This chapter presents the fundamental principles of orthogonality, weighted inner products, and polynomial approximation using orthogonal basis functions. These concepts serve as the foundation for the advanced spectral methods discussed in later chapters.

1.2 Orthogonality with Respect to a Weight Function

We denote by $w(x)$ a non-negative weight function defined on the closed interval $[a, b]$. Two functions f(x) and g(x) are defined to be orthogonal with respect to the weight function $w(x)$ if

$$\int_a^b f(x)\, g(x)\, w(x)\, dx = 0. \tag{1.1}$$

Let $w(x)$ be a weight function over [a,b]. A sequence of polynomials $\{P_n(x)\}_{n=0}^{\infty}$ is called an orthogonal polynomial system on $[a, b]$ associated with $w(x)$,Whenever

$$\int_a^b P_m(x)\, P_n(x)\, w(x)\, dx = 0, \quad \text{for } m \neq n. \tag{1.2}$$

This concept extends the notion of orthogonality from vectors in Euclidean space to functions in infinite-dimensional spaces.

1.3 Weighted Inner Product and Function Spaces

The weighted inner product associated with two functions $f(x)$ and $g(x)$ is defined by

$$\langle f, g \rangle = \int_a^b f(x)\, g(x)\, w(x)\, dx. \tag{1.3}$$

Using this definition, the collection of square-integrable functions on the interval $[a, b]$ with respect to the weight $w(x)$ forms a Hilbert space, denoted by $L^2_w(a, b)$. Orthogonal polynomials serve as a basis for this space, enabling the representation of functions as infinite or finite series expansions.

1.4 Approximation Using Orthogonal Polynomials

Let $f(x) \in L^2_w(a, b)$. Then $f(x)$ may be approximated using a finite expansion of orthogonal polynomials as

$$f(x) \approx \sum_{n=0}^{N} c_n P_n(x), \tag{1.4}$$

where the coefficients c_n are given by

$$c_n = \frac{\langle f, P_n \rangle}{\langle P_n, P_n \rangle}. \tag{1.5}$$

This approximation minimizes the mean square error

$$\int_a^b |f(x) - p_N(x)|^2 w(x)\, dx, \tag{1.6}$$

where $p_N(x)$ denotes a polynomial whose degree does not exceed N.

1.5 Three-Term Recurrence Relation

One of the main structural properties of orthogonal polynomials is that they follow a three-term recurrence relation.

[Three-Term Recurrence Relation]

we denote by $\{P_n(x)\}$ a sequence of orthogonal polynomials for a positive weight function $w(x)$ on the interval $[a, b]$. Then it holds that there are real constants α_n and positive constants β_n such that

$$xP_n(x) = P_{n+1}(x) + \alpha_n P_n(x) + \beta_n P_{n-1}(x), \quad n \geq 1,$$

with initial conditions $P_0(x) = 1$ and $P_1(x) = x - \alpha_0$.

Proof. Since $P_n(x)$ is a polynomial of degree n, the product $xP_n(x)$ is a polynomial of degree $n+1$. Hence, it can be expressed as a linear combination of the orthogonal basis:

$$xP_n(x) = \sum_{k=0}^{n+1} c_k P_k(x).$$

Taking inner products with $P_m(x)$ and using orthogonality, all coefficients vanish except for $m = n+1, n, n-1$. This leads to the stated three-term recurrence relation, where $\beta_n > 0$ follows from the positivity of the inner product. □

The three-term recurrence relation is central to numerical computation of orthogonal polynomials and plays a key role in Gaussian quadrature and spectral approximation methods.

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1.6 Classical Families of Orthogonal Polynomials

1. Legendre Polynomials

The Legendre polynomials $\{P_n(x)\}$ form an orthogonal system on the interval $[-1, 1]$ with respect to the constant weight function $w(x) = 1$, that is,

$$\int_{-1}^{1} P_m(x)P_n(x)\,dx = 0, \quad m \neq n.$$

These polynomials arise in boundary value problems and potential theory, particularly in problems with spherical symmetry.

2. Chebyshev Polynomials

The Chebyshev polynomials $\{T_n(x)\}$ are orthogonal on the interval $[-1, 1]$ with the weight function

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

They satisfy the minimax property, which ensures that the maximum deviation between a function and its polynomial approximation is minimized. Consequently, Chebyshev polynomials are widely used in numerical interpolation and spectral methods.

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3. Hermite Polynomials

Hermite polynomials are orthogonal on the interval $(-\infty, \infty)$ with respect to the weight function $w(x) = e^{-x^2}$:

$$\int_{-\infty}^{\infty} H_m(x)H_n(x)e^{-x^2}\,dx = 0, \quad m \neq n.$$

These polynomials play an important role in probability theory and quantum mechanics, especially in the study of Gaussian distributions and harmonic oscillators.

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4. Laguerre Polynomials

Laguerre polynomials are orthogonal on $[0, \infty)$ with respect to the weight function $w(x) = e^{-x}$:

$$\int_{0}^{\infty} L_m(x)L_n(x)e^{-x}\,dx = 0, \quad m \neq n.$$

They are frequently used in problems involving exponential decay, such as control theory and quantum mechanical systems.

1.7 Central Problem of Approximation Theory Using Orthogonal Series

Approximation theory is concerned with representing a given function by simpler functions, such as polynomials,such that the error of approximation is minimized in a prescribed norm. In many practical applications, an exact representation of the function is neither possible nor necessary. Instead, the goal is to obtain an accurate and computationally efficient approximation using a finite number of terms. Orthogonal polynomials provide a natural and powerful framework for addressing this problem.

Let $f(x)$ be a function defined on an interval $[a, b]$, and let $\{P_n(x)\}_{n=0}^{\infty}$ be a sequence of polynomials orthogonal with respect to a positive weight function $w(x)$. The central problem of approximation theory may be stated as follows: to determine a polynomial $p_n(x)$ of degree at most n such that the error

$$\|f - p_n\|$$

is minimized in a given norm.

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1.7.1 Approximation in the L^2 Norm

The approximation error is measured in the L^2 norm in a mean-square sense, and is defined as

$$\|f - p_n\|_{L^2} = \left(\int_a^b |f(x) - p_n(x)|^2 w(x)\, dx \right)^{1/2}.$$

The best approximation in the L^2 norm is obtained by projecting the function $f(x)$ onto the finite-dimensional subspace spanned by the first $n + 1$ orthogonal polynomials. This yields the approximation

$$p_n(x) = \sum_{k=0}^{n} c_k P_k(x), \quad c_k = \frac{\langle f, P_k \rangle}{\langle P_k, P_k \rangle}.$$

This representation is called a Fourier series in orthogonal polynomials. The partial sum $p_n(x)$ is the best polynomial of degree not exceeding n in the mean square sense. These types of approximations are widely used in numerical analysis and signal processing, where the most important thing is to reduce the average error. —

1.7.2 Approximation in the L^∞L-infinity Norm

In the L^∞ norm, the error is measured by the maximum deviation between the function and its approximation and is defined as

$$\|f - p_n\|_\infty = \max_{x \in [a,b]} |f(x) - p_n(x)|.$$

This form of approximation is particularly important in applications where uniform accuracy over the entire interval is required. Unlike the L^2 norm, the best approximation in the sense of L^∞ is generally harder to achieve.

Chebyshev polynomials provide near-optimal solutions to this problem due to their minimax property, which ensures that the maximum approximation error is minimized and distributed as evenly as possible over the interval. Consequently, Chebyshev polynomial approximations form the basis of minimax approximation theory and are extensively used in interpolation and spectral methods.

1.8 Key Concepts in Approximation Theory

This section introduces the main concepts that form the theoretical basis of approximation theory, namely the Gram matrix, normal equations and the qualitative Weierstrass Approximation Theorem. These ideas illustrate how polynomial approximations are built up , and explain why such an approximation is mathematically justified .

1. Gram Matrix

Let $\{\phi_1(x), \phi_2(x), \ldots, \phi_n(x)\}$ be a collection of functions defined on an interval $[a, b]$ with respect to a weight function $w(x)$. The *Gram matrix* G associated with this set is defined by

$$G_{ij} = \langle \phi_i, \phi_j \rangle = \int_a^b \phi_i(x)\phi_j(x)w(x)\,dx, \quad i, j = 1, 2, \ldots, n.$$

The Gram matrix measures the pairwise inner products of the basis functions. If the functions $\{\phi_i\}$ are linearly independent, then the Gram matrix is symmetric and positive definite. In the special case when the basis functions are orthogonal, the Gram matrix becomes diagonal, which significantly simplifies approximation problems.

2. Normal Equations

Consider the problem of approximating a given function $f(x)$ using a linear combination of basis functions:

$$p(x) = \sum_{k=1}^{n} a_k \phi_k(x).$$

The coefficients a_k are selected so that the squared error in the L^2 sense is minimized:

$$\|f - p\|_{L^2}^2 = \int_a^b |f(x) - p(x)|^2 w(x)\,dx.$$

Minimization of this error leads to a system of linear equations known as the *normal equations*:

$$\sum_{k=1}^{n} a_k \langle \phi_k, \phi_j \rangle = \langle f, \phi_j \rangle, \quad j = 1, 2, \ldots, n.$$

The normal equations can be written in matrix form:

$$G\mathbf{a} = \mathbf{b},$$

where G is the Gram matrix, $\mathbf{a} = (a_1, a_2, \ldots, a_n)^T$ is the vector of unknown coefficients, and

$\mathbf{b} = (\langle f, \phi_1 \rangle, \langle f, \phi_2 \rangle, \ldots, \langle f, \phi_n \rangle)^T$.

When orthogonal polynomials are used as basis functions, the Gram matrix is diagonal, and the normal equations decouple, making the computation of coefficients straightforward.

3. Weierstrass Approximation Theorem

[Weierstrass Approximation Theorem] The Weierstrass Approximation Theorem states that if $f(x)$ is continuous on a closed and bounded interval $[a, b]$. Then, for every $\varepsilon > 0$, there exists a polynomial $p(x)$ such that

$$\max_{x \in [a,b]} |f(x) - p(x)| < \varepsilon.$$

This theorem is qualitative in nature because it guarantees the existence of a polynomial approximation without explicitly constructing one. Even so, it provides the theoretical basis for polynomial approximation in the uniform norm and serves as a cornerstone of approximation theory.

1.9 Real-Life Applications

1. Signal Processing

In signal denoising, a noisy signal can be approximated using orthogonal polynomial expansions. By truncating higher-order terms, noise components are filtered out while preserving the essential structure of the signal.

2. Data Compression

Orthogonal polynomial approximations allow efficient representation of data using fewer coefficients. This principle is widely used in data compression, image processing, and spectral methods.

3. Physics and Engineering

Orthogonal polynomials appear in many physical models, such as:

- Quantum mechanics (Hermite polynomials in harmonic oscillators),
- Heat transfer and vibration analysis,
- Numerical solutions of differential equations using spectral methods.

4. Importance of Orthogonality in Approximation

The orthogonality property ensures:

- Unique determination of expansion coefficients,
- Reduction of approximation error,
- Numerical stability in computations,
- Faster convergence of approximation series.

These advantages make orthogonal polynomial approximation superior to ordinary polynomial interpolation in many applications.

Chapter 2

Classical Polynomial Families and Their Approximation Properties

2.1 Introduction

Approximation by orthogonal polynomials is a central topic in approximation theory and numerical analysis, and it offers efficient and stable ways to approximate complex functions through polynomial expansions. The use of orthogonal bases ensures desirable properties such as convergence, error minimization, and numerical stability, which are essential in scientific computing and applied mathematics.

This chapter focuses on the classical families of orthogonal polynomials and their approximation properties. In particular, Chebyshev polynomials of the first kind are examined for their optimal uniform approximation behavior. Their minimax property guarantees the smallest possible maximum error, while the explicit distribution of their roots and extrema leads to highly stable interpolation schemes. These features make Chebyshev polynomials especially effective for approximating smooth functions on finite intervals.

Legendre polynomials are orthogonal for a constant weight on the interval $[-1, 1]$ and are well suited for least squares approximation. They provide optimal approximations in the $L^2[-1, 1]$ norm and are widely used in problems where minimizing the mean-square error is of primary importance. For approximation on unbounded domains, Hermite and Laguerre polynomials form appropriate bases, corresponding respectively to the entire real line and the semi-infinite interval $[0, \infty)$, and are particularly effective for functions with rapid decay.

The chapter also highlights the role of weight functions, differential equations, and explicit polynomial representations in determining approximation efficiency. A comparative discussion is presented to illustrate the suitability of each polynomial family for different classes of functions. The close connection between orthogonal polynomials and Gaussian quadrature rules is also emphasized, underscoring their importance in numerical integration and computational methods.

2.2 Chebyshev Polynomials of the First Kind

The Chebyshev polynomials of the first kind, $T_n(x)$, are defined on the interval $[-1, 1]$ using trigonometric representation

$$T_n(x) = \cos(n \arccos x), \quad x \in [-1, 1], \; n = 0, 1, 2, \ldots \tag{2.1}$$

These polynomials satisfy the recurrence relation

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad n \geq 1, \tag{2.2}$$

with initial conditions $T_0(x) = 1$ and $T_1(x) = x$.

Orthogonality Property: Chebyshev polynomials of the first kind are orthogonal over the interval $[-1, 1]$ when measured using the weight function

$$w(x) = \frac{1}{\sqrt{1 - x^2}} \tag{2.3}$$

The orthogonality condition is given by

$$\int_{-1}^{1} T_m(x)T_n(x)\, w(x)\, dx = \begin{cases} 0, & m \neq n, \\ \frac{\pi}{2}, & m = n \neq 0, \\ \pi, & m = n = 0. \end{cases} \tag{2.4}$$

This orthogonality ensures numerical stability and efficiency when Chebyshev polynomials are used as basis functions in approximation problems.

2.3 Minimax Property of Chebyshev Polynomials

One of the most important properties of Chebyshev polynomials is their minimax or best uniform approximation property. Among monic polynomials of degree n, the scaled Chebyshev polynomial

$$\frac{1}{2^{n-1}} T_n(x) \tag{2.5}$$

minimizes the maximum absolute value on the interval $[-1, 1]$, that is,

$$\min_{p_n} \max_{x \in [-1,1]} |p_n(x)|, \tag{2.6}$$

where $p_n(x)$ is any polynomial of degree n.

This property implies that Chebyshev polynomial approximations yield the smallest possible maximum error and are therefore optimal in the uniform norm. This makes them particularly useful in numerical algorithms requiring high accuracy.

2.4 Roots and Extrema of Chebyshev Polynomials

For the Chebyshev polynomial $T_n(x)$, the roots are obtained as

$$x_k = \cos\left(\frac{(2k-1)\pi}{2n}\right), \quad k = 1, 2, \ldots, n. \tag{2.7}$$

These roots are known as *Chebyshev nodes*. They are non-uniformly distributed and cluster near the endpoints of the interval $[-1, 1]$. Interpolation at these nodes significantly reduces oscillations near the boundaries and avoids the Runge phenomenon commonly observed with equally spaced interpolation points.

The extrema of $T_n(x)$ occur at

$$x_k = \cos\left(\frac{k\pi}{n}\right), \quad k = 0, 1, \ldots, n, \tag{2.8}$$

where the polynomial attains the values

$$T_n(x_k) = (-1)^k. \tag{2.9}$$

The equal oscillation of Chebyshev polynomials between -1 and 1 at these extrema provides a geometric explanation of their minimax property.

2.5 Chebyshev Interpolation

Assume that $f(x)$ is a continuous function defined on the interval $[-1, 1]$. The Chebyshev interpolation polynomial $P_n(x)$ is obtained by evaluating the function at Chebyshev nodes.Compared with interpolation based on uniformly spaced points,this method generally produces much better accuracy.

If the function $f(x)$ satisfies suitable smoothness conditions , the interpolaion error can be bounded as

$$\|f - P_n\|_\infty \leq C\frac{\|f^{(n+1)}\|_\infty}{2^{n-1}}, \tag{2.10}$$

where C denotes a positive constant.This estimate indicates that Chebyshev interpolation converges rapidly for sufficiently smooth functions.

Illustrative Example: suppose we have the function

$$f(x) = \frac{1}{1 + 25x^2}, \quad x \in [-1, 1]. \tag{2.11}$$

When interpolation is carried out using equally spaced nodes, the resulting polynomial often develops significant oscillations near the endpoints of the interval, a phenomenon commonly referred to as the Runge phenomenon. In contrast, interpolation based on Chebyshev nodes produces a polynomial that approximates the function much more accurately over the entire interval while considerably reducing the maximum error.

This example highlights the practical efficiency of Chebyshev interpolation techniques in approximation problems.

2.6 Legendre Polynomials and $L^2[-1,1]$ Approximation

Legendre polynomials form one of the most important families of classical orthogonal polynomials and play a major role in approximation theory, especially in least-square approximation problems on bounded intervals. These polynomials arise from the orthogonality relation defined on the interval $[-1,1]$ with respect to the constant weight function $w(x) = 1$.

The sequence of Legendre polynomials $\{P_n(x)\}_{n=0}^{\infty}$ satisfies the orthogonality condition

$$\int_{-1}^{1} P_m(x)\,P_n(x)\,dx = 0, \quad m \neq n. \tag{2.12}$$

This property makes Legendre polynomials particularly suitable for approximating functions belonging to the Hilbert space $L^2[-1,1]$.

A standard explicit expression for Legendre polynomials is given through Rodrigues' formula:

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left[(x^2-1)^n\right], \quad n = 0, 1, 2, \ldots \tag{2.13}$$

The first few Legendre polynomials are

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \frac{1}{2}(3x^2 - 1). \tag{2.14}$$

From the perspective of approximation theory, Legendre polynomials yield the best approximation in the mean-square sense. Any function $f \in L^2[-1,1]$ may be represented through a Legendre polynomial expansion of the form

$$f(x) \approx \sum_{n=0}^{N} a_n P_n(x), \tag{2.15}$$

where the coefficients a_n are obtained by means of orthogonal projection:

$$a_n = \frac{2n+1}{2}\int_{-1}^{1} f(x)\,P_n(x)\,dx. \tag{2.16}$$

This representation gives the smallest possible error in the L^2 sense namely,

$$\|f - S_N\|_2 = \min_{p \in \mathcal{P}_N} \|f - p\|_2, \tag{2.17}$$

where S_N denotes the partial sum up to degree N , and $\mathcal{P}_N$ represents the collection of all polynomial whose degree does not exceed N.

The convergence behavior of Legendre polynomial approximations depends strongly on the smoothness of the function being approximated. For smooth or analytic functions, the Legendre coefficients decay rapidly, resulting in highly accurate approximations using relatively few terms. This property is extensively exploited in numerical analysis, particularly in spectral methods for solving ordinary and partial differential equations.

Legendre polynomial approximations are widely used in physics and engineering applications involving bounded domains. Typical applications include potential theory, quantum mechanics, and signal approximation problems defined on finite intervals. Their optimality in the least-squares sense makes them especially suitable for applications where average error minimization is of primary importance.

In conclusion, Legendre polynomials provide a mathematically rigorous and computationally efficient framework for function approximation in $L^2[-1,1]$. Their orthogonality, explicit construction, and optimal approximation properties establish them as a cornerstone of classical approximation theory.

2.7 Hermite and Laguerre Polynomials for Unbounded Domains

In many mathematical, physical, and engineering applications, functions are often defined over unbounded intervals such as $(-\infty,\infty)$ or $[0,\infty)$. To deal with approximation problems on such domains, special orthogonal polynomial families including Hermite and Laguerre polynomials are employed. Unlike polynomial systems designed for finite intervals, these families incorporate exponentially decaying weight functions, which ensure stability and convergence across infinite domains.

2.7.1 Hermite Polynomials

The sequence of Hermite polynomials $\{H_n(x)\}_{n=0}^{\infty}$ forms an orthogonal system on the interval $(-\infty,\infty)$ with respect to the Gaussian weight function

$$w(x) = e^{-x^2}. \tag{2.18}$$

The orthogonality property of Hermite polynomials is expressed as

$$\int_{-\infty}^{\infty} H_m(x)\, H_n(x)\, e^{-x^2}\, dx = 0, \quad m \neq n. \tag{2.19}$$

An explicit formula for generating Hermite polynomials is given through Rodrigues' formula:

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}\left(e^{-x^2}\right), \quad n = 0, 1, 2, \ldots \tag{2.20}$$

The first few Hermite polynomials are

$$H_0(x) = 1, \quad H_1(x) = 2x, \quad H_2(x) = 4x^2 - 2. \tag{2.21}$$

Hermite polynomials satisfy the second-order linear differential equation

$$y'' - 2xy' + 2ny = 0, \tag{2.22}$$

which naturally appears in several branches of mathematical physics. In particular,these polynomials play an important role in describing the one -dimensional quantum harmonic oscillator

From the perspective of approximation-theory, any function f satisfying

$$\int_{-\infty}^{\infty} |f(x)|^2 e^{-x^2}\, dx < \infty \tag{2.23}$$

can be represented approximatey by a Hermite series of the form

$$f(x) \approx \sum_{n=0}^{N} a_n H_n(x), \tag{2.24}$$

where the coefficients a_n are determined using orthogonal projection:

$$a_n = \frac{1}{\|H_n\|^2} \int_{-\infty}^{\infty} f(x)\, H_n(x)\, e^{-x^2}\, dx. \tag{2.25}$$

Hermite polynomial approximations are particularly effective for functions exhibiting Gaussian-type decay.

2.7.2 Laguerre Polynomials

Laguerre polynomials $\{L_n(x)\}_{n=0}^{\infty}$ form an orthogonal system on the semi-infinite interval $[0, \infty)$ with respect to the exponential weight function

$$w(x) = e^{-x}. \tag{2.26}$$

Their orthogonality relation is given by

$$\int_0^{\infty} L_m(x)\, L_n(x)\, e^{-x}\, dx = 0, \quad m \neq n. \tag{2.27}$$

Laguerre polynomials admit the Rodrigues' formula

$$L_n(x) = \frac{e^x}{n!} \frac{d^n}{dx^n} \left(e^{-x} x^n \right), \quad n = 0, 1, 2, \ldots \tag{2.28}$$

The first few Laguerre polynomials are

$$L_0(x) = 1, \quad L_1(x) = 1 - x, \quad L_2(x) = \frac{1}{2}(x^2 - 4x + 2). \tag{2.29}$$

Laguerre polynomials satisfy the differential equation

$$xy'' + (1 - x)y' + ny = 0, \tag{2.30}$$

which frequently appears in problems with radial symmetry.

Any function f satisfying

$$\int_0^{\infty} |f(x)|^2 e^{-x}\, dx < \infty \tag{2.31}$$

may be approximated through a Laguerre series expansion of the form

$$f(x) \approx \sum_{n=0}^{N} b_n L_n(x), \tag{2.32}$$

where the coefficients b_n are given by

$$b_n = \frac{1}{\|L_n\|^2} \int_0^{\infty} f(x)\, L_n(x)\, e^{-x}\, dx. \tag{2.33}$$

Laguerre polynomial approximations are particularly useful in modeling decay processes and problems defined on semi-infinite domains.

2.8 Comparative Analysis of Classical Orthogonal Polynomials and Gaussian Quadrature

Classical orthogonal polynomial families, including Chebyshev, Legendre, Hermite, and Laguerre polynomials, occupy an important position in approximation theory. Their effectiveness largely depends on the characteristics of the function being approximated. This section provides a comparative discussion of these polynomial families for different categories of functions and also examines their relationship with Gaussian quadrature methods.

2.8.1 Criteria for Approximation Efficiency

Suppose a function $f(x)$ be approximated by

$$f(x) \approx \sum_{n=0}^{N} a_n P_n(x),$$

where $P_n(x)$ are orthogonal polynomials. The efficiency of approximation depends on:

- Rate of convergence
- Stability of interpolation
- Ability to handle singularities
- Suitability for domain (bounded or unbounded)
- Numerical conditioning

2.8.2 Approximation of Smooth Functions:

1. Chebyshev Polynomials

For smooth functions $f \in C^{\infty}([-1,1])$, Chebyshev coefficients decay exponentially:

$$|a_n| = O(e^{-cn}),$$

for some $c > 0$. This leads to spectral convergence.

Chebyshev polynomials are optimal in the uniform norm due to their minimax property and provide excellent numerical stability because of clustering of interpolation points near the endpoints.

2. Legendre Polynomials

Legendre polynomials are optimal in the $L^2[-1,1]$ norm. For $f \in C^k([-1,1])$,

$$|a_n| = O(n^{-k}).$$

Thus, convergence is algebraic rather than exponential.

Comparison:

- Chebyshev: best for uniform approximation
- Legendre: best for L^2 approximation and variational problems

Hermite and Laguerre Polynomials

For unbounded domains:

- Hermite polynomials: domain $(-\infty, \infty)$ with weight e^{-x^2}
- Laguerre polynomials: domain $[0, \infty)$ with weight e^{-x}

For smooth and rapidly decaying functions, the coefficients decay exponentially, leading to efficient approximations.

2.8.3 Approximation of Periodic Functions

Using the transformation

$$x = \cos\theta,$$

Chebyshev expansions become equivalent to cosine Fourier series. Thus, Chebyshev polynomials are highly effective for periodic functions defined on finite intervals.

2.8.4 Approximation of Functions with Singularities

Endpoint Singularities

Take a function expressed as :

$$f(x) = (1-x)^\alpha.$$

Chebyshev polynomials perform better than Legendre polynomials due to node clustering near endpoints. However, convergence becomes algebraic rather than exponential.

Interior Singularities

For functions with discontinuities:

- All polynomial approximations exhibit Gibbs phenomenon
- Coefficients decay slowly:

$$|a_n| = O(n^{-1})$$

Comparative Summary

Feature	Chebyshev	Legendre	Hermite	Laguerre
Domain	$[-1,1]$	$[-1,1]$	$\mathbb{R}$	$[0,\infty)$
Weight	$(1-x^2)^{-1/2}$	1	e^{-x^2}	e^{-x}
Best for	Uniform approx	L^2 approx	Decaying functions	Semi-infinite problems
Convergence	Exponential	Algebraic	Exponential	Exponential

2.9 Connection with Gaussian Quadrature Rules

Gaussian quadrature is one of the most powerful numerical techniques for approximating definite integrals of the form

$$I = \int_a^b f(x)w(x)\,dx,$$

where $w(x)$ denotes a prescribed weight function. Unlike classical Newton–Cotes formulas, Gaussian quadrature selects optimal nodes and weights to maximize the degree of exactness.

The quadrature formula is given by

$$I \approx \sum_{i=1}^{n} w_i f(x_i),$$

where x_i are the quadrature nodes and w_i are the associated weights.

Role of Orthogonal Polynomials

Let $\{P_n(x)\}$ be a sequence of orthogonal polynomials with respect to the weight function $w(x)$ over the interval $[a, b]$, satisfying

$$\int_a^b P_m(x)P_n(x)w(x)\,dx = 0, \quad m \neq n.$$

The central principle behind Gaussian quadrature is as follows:

- The nodes x_i are selected as the zeros of the orthogonal polynomial $P_n(x)$.
- The weights w_i are chosen so that the quadrature rule becomes exact for polynomials of the highest achievable degree.

Degree of Exactness: An n -point Gaussian quadrature rule integrates exactly every polynomial of degree at most $2n - 1$, i.e.,

$$\int_a^b p(x)w(x)\,dx = \sum_{i=1}^{n} w_i p(x_i),$$

for all polynomials $p(x)$ with $\deg(p) \leq 2n - 1$.

This optimality distinguishes Gaussian quadrature from other numerical integration methods.

2.9.1 Classical Gaussian Quadrature Rules

Gauss–Legendre Quadrature

- Interval: $[-1, 1]$
- Weight function: $w(x) = 1$
- Nodes: roots of Legendre polynomials $P_n(x)$

The quadrature rule is

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{i=1}^{n} w_i f(x_i).$$

Gauss–Chebyshev Quadrature

- Interval: $[-1, 1]$
- Weight function: $w(x) = \frac{1}{\sqrt{1-x^2}}$

The nodes are

$$x_i = \cos\left(\frac{2i-1}{2n}\pi\right),$$

Thus,the quadrature expression can be written as

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx \approx \frac{\pi}{n} \sum_{i=1}^{n} f(x_i).$$

Gauss–Hermite Quadrature

- Interval: $(-\infty, \infty)$
- Weight function: $w(x) = e^{-x^2}$
- Nodes: roots of Hermite polynomials

$$\int_{-\infty}^{\infty} f(x) e^{-x^2} dx \approx \sum_{i=1}^{n} w_i f(x_i).$$

Gauss–Laguerre Quadrature

- Interval: $[0, \infty)$
- Weight function: $w(x) = e^{-x}$
- Nodes: roots of Laguerre polynomials

$$\int_{0}^{\infty} f(x) e^{-x} dx \approx \sum_{i=1}^{n} w_i f(x_i).$$

Error Analysis

If $f \in C^{2n}[a,b]$, then the error in Gaussian quadrature is formulated as

$$E_n(f) = \frac{f^{(2n)}(\xi)}{(2n)!} \int_a^b \prod_{i=1}^{n} (x - x_i)^2 w(x)\, dx,$$

for some $\xi \in (a,b)$.

This shows that the error depends on higher-order derivatives of f, leading to rapid convergence for smooth functions.

Comparative Analysis

Different orthogonal polynomial families yield Gaussian quadrature rules adapted to specific domains:

Polynomial	Interval	Weight Function	Application
Legendre	$[-1, 1]$	1	Smooth functions
Chebyshev	$[-1, 1]$	$(1 - x^2)^{-1/2}$	Endpoint singularities
Hermite	$(-\infty, \infty)$	e^{-x^2}	Rapid decay functions
Laguerre	$[0, \infty)$	e^{-x}	Exponential decay

Chapter 3

Convergence and Error Analysis of Orthogonal Series

3.1 Introduction

Orthogonal polynomial approximations play a central role in both theoretical and applied mathematics because of their efficiency in representing complex functions. Earlier chapters mainly focused on the construction and fundamental properties of orthogonal polynomial systems. In this chapter, the emphasis shifts toward understanding how accurately these expansions approximate a function and how the approximation error behaves as the degree of the polynomial increases.This chapter focuses on a detailed examination of this problem,which can be summarized through the following question:

> *How fast does the approximation error tend to zero as the degree of approximation increases?*

To address this quantitative problem, the chapter examines the convergence behavior of orthogonal polynomial series and provides precise estimates for the approximation error associated with finite partial sums. Given a function f and its orthogonal expansion with respect to a classical polynomial system, the degree-n partial sum $S_n(f)$ serves as a polynomial approximation of f. The central object of study is therefore the error term

$$f(x) - S_n(f)(x),$$

whose decay rate, normwise behavior, and pointwise structure are analyzed in detail.

A key aspect of approximation theory is the relationship between the smoothness of a function and the speed of convergence of its polynomial approximation. Classical results, especially those related to Jackson-type theorems, demonstrate that smoother functions generally produce faster convergence rates. Functions possessing higher-order derivatives tend to exhibit rapidly decreasing approximation errors, whereas functions with limited smoothness usually converge at a slower rate. On the other hand, analytic functions often display exponential convergence when approximated through orthogonal polynomial expansions.

In addition to global error estimates, this chapter investigates the asymptotic behavior of the expansion coefficients in orthogonal series. The decay rate of these coefficients provides valuable insight into convergence mechanisms and serves as an indicator of approximation quality. Smooth functions are characterized by rapidly decaying coefficients, whereas non-smooth functions generate slowly decaying coefficients, directly affecting the effectiveness of polynomial approximation.

The chapter also examines approximation methods based on interpolation, with particular attention given to interpolation at the zeros of orthogonal polynomials, especially Chebyshev nodes. In this setting, the Lebesgue constant is an important tool for evaluating the stability and reliability of interpolation methods. The relatively slow growth of the Lebesgue constant in Chebyshev interpolation explains why it performs better than interpolation at equally spaced points, where numerical instability and larger approximation errors are more likely to occur.

A major limitation of orthogonal polynomial approximation is highlighted through the study of the *Gibbs phenomenon*, which occurs when approximating functions with jump discontinuities. Although convergence is achieved away from points of discontinuity, persistent oscillations appear in their neighborhood, and the maximum overshoot does not vanish as the degree of approximation increases. This phenomenon illustrates that convergence in norm does not necessarily imply uniform or pointwise convergence and underscores the intrinsic challenges of approximating non-smooth functions.

To clarify these theoretical results, illustrative examples are discussed throughout the chapter. For instance, the approximation of piecewise-defined functions using Chebyshev or Legendre polynomials demonstrates both the high accuracy achievable for smooth regions and the emergence of oscillatory behavior near discontinuities. Such examples bridge the gap between abstract theoretical results and practical approximation behavior.

Overall, this chapter presents a detailed study of convergence and error analysis for orthogonal polynomial approximations. By combining ideas from approximation theory, stability analysis, and convergence results, the chapter develops a solid framework for understanding the capabilities and limitations of orthogonal series. The discussions presented here also provide a strong foundation for advanced numerical techniques, spectral methods, and further developments in approximation theory.

3.2 Rate of Convergence of Approximation Error

A fundamental question is how fast the approximation error $\|f - S_n(f)\|$ tends to zero as $n \to \infty$.

3.2.1 General Principle

The speed of convergence is closely related to the smoothness of the function:

- If $f \in L^2$, then $S_n(f) \to f$ in mean square sense.
- If f is continuous, convergence may be pointwise.
- If $f \in C^k$, then convergence is faster.

Example: Chebyshev Expansion

For Chebyshev polynomial expansions:

- If $f \in C^k[-1,1]$, then
$$|a_n| = O(n^{-k-1}).$$
- If f is analytic, then
$$|a_n| = O(\rho^{-n}), \quad \rho > 1.$$

Thus, smoother functions lead to faster convergence.

3.3 Jackson-Type Theorems for Algebraic Polynomials

Jackson-type theorems provide quantitative estimates of approximation error.

Statement

Suppose $f \in C[-1,1]$. Then there is a polynomial p_n whose degree does not exceed n such that

$$\|f - p_n\|_\infty \leq C\,\omega\left(f, \frac{1}{n}\right),$$

where $\omega(f,\delta)$ denotes the modulus of continuity defined by:

$$\omega(f,\delta) = \sup_{|x-y|\leq\delta} |f(x) - f(y)|.$$

Proof. The proof proceeds in several steps.

Step 1: Reduction to periodic functions.

Define a change of variable:

$$x = \cos\theta, \quad \theta \in [0,\pi].$$

Then define

$$g(\theta) = f(\cos\theta),$$

which extends to an even 2π-periodic function.

Step 2: Approximation via convolution.

We approximate g using the Jackson kernel $J_n(\theta)$:

$$g_n(\theta) = \frac{1}{\pi}\int_{-\pi}^{\pi} g(\theta - t) J_n(t)\,dt.$$

The Jackson kernel satisfies:

- $J_n(t) \geq 0$
- $\frac{1}{\pi}\int_{-\pi}^{\pi} J_n(t)\,dt = 1$
- Concentration near $t = 0$

Step 3: Error estimate.

We estimate:

$$|g(\theta) - g_n(\theta)| \leq \frac{1}{\pi}\int_{-\pi}^{\pi} |g(\theta) - g(\theta - t)| J_n(t)\,dt.$$

Using the modulus of continuity:

$$|g(\theta) - g(\theta - t)| \leq \omega(g, |t|),$$

we obtain:

$$|g(\theta) - g_n(\theta)| \leq \frac{1}{\pi} \int_{-\pi}^{\pi} \omega(g, |t|) J_n(t)\, dt.$$

Since $J_n(t)$ is concentrated near $t = 0$, we estimate:

$$|g(\theta) - g_n(\theta)| \leq C\, \omega \left(g, \frac{1}{n} \right).$$

Step 4: to algebraic polynomials.

The function $g_n(\theta)$ is a trigonometric polynomial of degree n. Thus,

$$p_n(x) := g_n(\arccos x)$$

forms an algebraic polynomial whose degree is at most n.

Finally, since $\omega(g, \delta) \leq \omega(f, \delta)$, we obtain:

$$\|f - p_n\|_\infty \leq C\, \omega \left(f, \frac{1}{n} \right).$$

This establishes the required result. □

3.4 Higher Order Estimate

If the function $f \in C^k$, then the approximation error satisfies

$$\|f - p_n\| \leq \frac{C}{n^k} \|f^{(k)}\|.$$

This estimates shows that smoother functions generally admit more accurate polynomial approximations.

3.5 Lebesgue Constant and Interpolation at Orthogonal Nodes

Definition:

The Lebesgue constant Λ_n is defined as

$$\Lambda_n = \sup_{x \in [-1,1]} \sum_{k=0}^{n} |l_k(x)|,$$

where $l_k(x)$ denotes the Lagrange interpolation polynomials.

Error Estimate

The interpolation error satisfies the inequality

$$|f(x) - p_n(x)| \leq (1 + \Lambda_n) \inf_{p \in \Pi_n} \|f - p\|.$$

Chebyshev Nodes
For Chebyshev nodes:

$$\Lambda_n = O(\log n).$$

For equally spaced nodes:

$$\Lambda_n = O(2^n).$$

Thus, Chebyshev nodes provide significantly better stability.

3.6 Analysis of the Error Term $f(x) - S_n(f)(x)$

The approximation error can be represented as

$$f(x) - S_n(f)(x) = \sum_{k=n+1}^{\infty} a_k P_k(x).$$

Asymptotic Behavior
The convergence rate depends on the decay of coefficients:

- If $a_k \sim \frac{1}{k^2}$, then error is $O(1/n)$.
- If $a_k \sim e^{-k}$, then error is $O(e^{-n})$.

Types of Convergence

- L^2 convergence: always guaranteed.
- Uniform convergence: requires stronger smoothness conditions.

3.7 Gibbs Phenomenon for Non-Smooth Functions

Orthogonal polynomial expansions provide highly accurate approximations for smooth functions. However, when the target function possesses discontinuities or non-smooth behavior, the approximation exhibits characteristic oscillations near such points. This phenomenon is known as the **Gibbs phenomenon**.

Consider the orthogonal series expansion:

$$S_n(f)(x) = \sum_{k=0}^{n} a_k P_k(x),$$

where $\{P_k(x)\}$ is a system of orthogonal polynomials. While $S_n(f)(x)$ converges effectively for smooth functions, difficulties arise when f has discontinuities.

Nature of the Gibbs Phenomenon
Assume that the function $f(x)$ has a jump discontinuity at $x = x_0$. Then,

$$\lim_{x \to x_0^-} f(x) = f(x_0^-), \quad \lim_{x \to x_0^+} f(x) = f(x_0^+).$$

Define the jump magnitude:

$$J = f(x_0^+) - f(x_0^-).$$

The partial sums $S_n(f)(x)$ exhibit the following properties:

- At the point of discontinuity,

$$\lim_{n\to\infty} S_n(f)(x_0) = \frac{f(x_0^+) + f(x_0^-)}{2}.$$

- Near x_0, oscillations appear in the approximation.
- The maximum overshoot approaches approximately

$$0.08949 \times J,$$

i.e., about 9% of the jump.

Mathematical Explanation

The Gibbs phenomenon can be understood through the kernel representation of partial sums. In general, the approximation can be written as:

$$S_n(f)(x) = \int f(t)K_n(x,t)\,dt,$$

where $K_n(x,t)$ is an oscillatory kernel (e.g., Dirichlet kernel in Fourier analysis).

The kernel has the following properties:

- It oscillates with increasing frequency as n increases.
- It does not converge uniformly to a Dirac delta function.
- It exhibits large side lobes near discontinuities.

As a result, near a discontinuity, the integral accumulates oscillatory contributions, leading to persistent overshoots.

Behavior of the Error

Let the approximation error be defined as:

$$E_n(x) = f(x) - S_n(f)(x).$$

Then:

- Away from the discontinuity,

$$E_n(x) \to 0 \quad \text{as } n \to \infty.$$

- Near the discontinuity,

$$\sup |E_n(x)| \not\to 0.$$

- The width of the oscillatory region behaves like

$$O\left(\frac{1}{n}\right).$$

Thus, although the oscillations become more localized, their amplitude remains essentially constant.

Illustrative Example

Let us examine the following step function:

$$f(x) = \begin{cases} 1, & x > 0, \\ -1, & x < 0. \end{cases}$$

Its orthogonal expansion (e.g., Fourier or Chebyshev series) exhibits:

- Oscillations near $x = 0$,
- Persistent overshoot even for large n,
- Shrinking width but fixed amplitude of oscillations.

Chapter 4

Computational Aspects and Applications in Spectral Methods

4.1 Introduction

This chapter is devoted to the computational aspects of approximation by orthogonal polynomials and their application in spectral methods for solving differential equations. The primary objective is to bridge the gap between theoretical approximation results and their practical implementation by developing efficient and stable numerical techniques. In particular, we discuss algorithms for the rapid evaluation of orthogonal polynomial expansions, emphasizing recurrence-based methods and the Clenshaw algorithm, followed by efficient computation of expansion coefficients using discrete transforms, with special focus on Chebyshev polynomials and the use of the Fast Fourier Transform (FFT). The chapter also addresses the implementation of Gaussian quadrature as an optimal tool for numerical integration based on orthogonal polynomials. To illustrate the effectiveness of these methods, a detailed example based on the Chebyshev spectral collocation method is presented, demonstrating the phenomenon of exponential convergence for smooth solutions. Thus, this chapter provides a comprehensive computational framework linking orthogonal polynomial approximation with high-accuracy numerical methods for differential equations.

4.2 Efficient Evaluation of Orthogonal Polynomial Expansions

Problem Statement:

Let $\{P_n(x)\}_{n=0}^{\infty}$ be a system of orthogonal polynomials with respect to a weight function $w(x)$ on an interval $[a, b]$. A function $f(x)$ is approximated by the truncated series:

$$S_N(f)(x) = \sum_{n=0}^{N} a_n P_n(x)$$

The objective is to evaluate $S_N(f)(x)$ efficiently.

1. Recurrence-Based Evaluation

Orthogonal polynomials generally satisfy a three-term recurrence relation of the form:

$$P_{n+1}(x) = (\alpha_n x + \beta_n)P_n(x) - \gamma_n P_{n-1}(x), \quad n \geq 1$$

together with the initial conditions $P_0(x)$ and $P_1(x)$.

This allows sequential computation of polynomials up to degree N. However, this approach may introduce numerical instability for large N.

2. Clenshaw Algorithm

A more stable and efficient method is the Clenshaw algorithm, used to evaluate:

$$S_N(f)(x) = \sum_{n=0}^{N} a_n P_n(x)$$

Define backward recursion:

$$b_k(x) = a_k + (\alpha_k x + \beta_k)b_{k+1}(x) - \gamma_{k+1} b_{k+2}(x)$$

with terminal conditions:

$$b_{N+1}(x) = 0, \quad b_{N+2}(x) = 0$$

Then,

$$S_N(f)(x) = b_0(x)$$

Advantages:

- Computational complexity $O(N)$
- Avoids explicit computation of $P_n(x)$
- Numerically stable

4.3 Computing Coefficients via Discrete Transforms

Introduction

In spectral methods, a function $f(x)$ is commonly approximated by a finite expansion of orthogonal basis functions:

$$f(x) \approx S_N(f)(x) = \sum_{k=0}^{N} a_k \phi_k(x), \tag{4.1}$$

where $\{\phi_k(x)\}$ denotes the orthogonal basis set and a_k represents the associated expansion coefficients.

The coefficients are traditionally computed using projection integrals:

$$a_k = \frac{\langle f, \phi_k \rangle}{\langle \phi_k, \phi_k \rangle}. \tag{4.2}$$

However, direct computation is expensive, motivating the use of discrete transforms.

4.3.1 Discrete Transform Approach

The coefficients can be approximated using discrete nodes:

$$a_k \approx \sum_{j=0}^{N} f(x_j)\phi_k(x_j)w_j, \tag{4.3}$$

where x_j are collocation points and w_j are quadrature weights.

4.3.2 Chebyshev Polynomials

Chebyshev polynomials $T_n(x)$ are widely used due to their numerical stability. The approximation becomes:

$$f(x) \approx \sum_{k=0}^{N} a_k T_k(x). \tag{4.4}$$

The corresponding chebyshev collocation points are defined by:

$$x_j = \cos\left(\frac{\pi j}{N}\right), \quad j = 0, 1, \ldots, N. \tag{4.5}$$

The coefficients are computed as:

$$a_k = \frac{2}{N}\sum_{j=0}^{N} f(x_j)\cos\left(\frac{\pi k j}{N}\right). \tag{4.6}$$

4.3.3 FFT and Chebyshev Polynomials

Using the identity:

$$T_k(\cos\theta) = \cos(k\theta), \tag{4.7}$$

the Chebyshev expansion can be transformed into a cosine-series representation:

$$f(\cos\theta) \approx \sum_{k=0}^{N} a_k \cos(k\theta). \tag{4.8}$$

Thus, coefficient computation reduces to a Discrete Cosine Transform (DCT), which can be efficiently evaluated using the Fast Fourier Transform (FFT).

4.3.4 FFT-Based Algorithm

1. Compute Chebyshev nodes:

$$x_j = \cos\left(\frac{\pi j}{N}\right) \tag{4.9}$$

2. Evaluate $f(x_j)$
3. Form an even extension of the data
4. Apply FFT
5. Extract coefficients a_k

4.3.5 Computational Complexity

- Direct method: $O(N^2)$
- FFT-based method: $O(N \log N)$

4.3.6 Example: FFT with Chebyshev Polynomials

Consider:

$$f(x) = e^x, \quad x \in [-1, 1]. \tag{4.10}$$

Steps:

1. Compute nodes $x_j = \cos\left(\frac{\pi j}{N}\right)$
2. Evaluate $f_j = e^{x_j}$
3. Apply FFT
4. Extract coefficients

Due to smoothness, coefficients decay rapidly, demonstrating spectral convergence.

4.4 Gaussian Quadrature

4.4.1 Definition

Gaussian quadrature approximates integrals as:

$$\int_{-1}^{1} f(x)w(x)\,dx \approx \sum_{j=0}^{N} w_j f(x_j), \tag{4.11}$$

where x_j represents the quadrature nodes and w_j denotes the associated weights

4.4.2 Exactness Property

A key feature of Gaussian quadrature is that it produces exact results for all polynomials whose degree does not exceed $2N + 1$.

4.4.3 Gauss–Chebyshev Quadrature

For the weight $w(x) = \frac{1}{\sqrt{1-x^2}}$:

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx \approx \frac{\pi}{N} \sum_{j=1}^{N} f(x_j), \tag{4.12}$$

where:

$$x_j = \cos\left(\frac{2j-1}{2N}\pi\right). \tag{4.13}$$

4.4.4 Implementation in Spectral Methods

Gaussian quadrature is used to:

1. Compute coefficients:

$$a_k \approx \sum_{j=0}^{N} w_j f(x_j) \phi_k(x_j) \tag{4.14}$$

2. Evaluate integrals in PDEs

3. Construct system matrices

4.4.5 Advantages of Gaussian Quadrature

- High accuracy
- Exactness for high-degree polynomials
- Efficient computation

4.4.6 Combined Use of FFT and Quadrature

In practice:

- FFT provides fast coefficient computation
- Gaussian quadrature ensures accurate integration

4.4.7 Applications

These methods are used in:

- Partial differential equations
- Fluid dynamics
- Quantum mechanics
- Signal processing

4.5 Spectral Methods for Solving Differential Equations

Introduction Spectral methods are widely recognized as powerful numerical tools for solving differential equations with high accuracy. The fundamental concept involves approximating the unknown solution using a finite expansion of globally defined orthogonal basis functions.

Let $u(x)$ be defined on $[-1, 1]$. Then the spectral approximation is:

$$u(x) \approx u_N(x) = \sum_{k=0}^{N} a_k \phi_k(x), \tag{4.15}$$

where $\phi_k(x)$ denotes the orthogonal basis functions and a_k represents the unknown expansion coefficients.

Basic Formulation:

Assume the differential equation:

$$\mathcal{L}u(x) = f(x), \tag{4.16}$$

where $\mathcal{L}$ represents a differential operator.

Replacing $u(x)$ with its approximation:

$$\mathcal{L}\left(\sum_{k=0}^{N} a_k \phi_k(x)\right) = f(x). \tag{4.17}$$

The problem reduces to finding coefficients a_k.

4.5.1 Types of Spectral Methods

Galerkin Method The residual is made orthogonal to the basis functions:

$$\langle \mathcal{L}u_N - f, \phi_j \rangle = 0, \quad j = 0, 1, \ldots, N. \tag{4.18}$$

Collocation Method (Pseudospectral Method) In the collocation technique, the governing equation is satisfied exactly at selected discrete collocation points:

$$\mathcal{L}u_N(x_j) = f(x_j), \quad j = 0, 1, \ldots, N. \tag{4.19}$$

Tau Method Boundary conditions are incorporated by modifying the highest-order coefficients.

4.5.2 Choice of Basis Functions

Common choices include:

- **Chebyshev Polynomials**: Known for excellent numerical stability and the use of clustered collocation points near boundaries.
- **Legendre Polynomials**: Orthogonal polynomials corresponding to the weight function $w(x) = 1$

Example 1: Boundary Value Problem

Consider:

$$-u''(x) = f(x), \quad x \in [-1, 1], \tag{4.20}$$

subject to the boundary condition:

$$u(-1) = 0, \quad u(1) = 0. \tag{4.21}$$

Step 1: Approximation

$$u_N(x) = \sum_{k=0}^{N} a_k \phi_k(x). \tag{4.22}$$

Step 2: Apply Operator

$$-\sum_{k=0}^{N} a_k \phi_k''(x) = f(x). \tag{4.23}$$

Step 3: Collocation

$$-\sum_{k=0}^{N} a_k \phi_k''(x_j) = f(x_j). \tag{4.24}$$

This leads to the linear system:

$$A\mathbf{a} = \mathbf{f}, \tag{4.25}$$

where

$$A_{jk} = -\phi_k''(x_j). \tag{4.26}$$

Step 4: Boundary Conditions Impose:

$$u_N(-1) = 0, \quad u_N(1) = 0. \tag{4.27}$$

4.5.3 Spectral Differentiation

Derivatives are computed using a differentiation matrix:

$$u'(x_i) \approx \sum_{j=0}^{N} D_{ij} u(x_j). \tag{4.28}$$

Second derivatives:

$$u''(x_i) \approx \sum_{j=0}^{N} (D^2)_{ij} u(x_j). \tag{4.29}$$

Convergence
Spectral methods exhibit exponential convergence for smooth functions:

$$\|u - u_N\| \leq Ce^{-\alpha N}. \tag{4.30}$$

Advantages

- High accuracy
- Fast convergence
- Efficient for smooth problems

Limitations

- Gibbs phenomenon near discontinuities
- Dense matrices
- Difficult for complex geometries

Applications
Spectral methods are used in:

- Fluid dynamics
- Quantum mechanics
- Weather modeling
- Signal processing

4.6 A Detailed Example: Chebyshev Spectral Collocation Method and Exponential Convergence

To demonstrate the effectiveness of spectral methods, consider a boundary value problem solved using the Chebyshev spectral collocation method. This example demonstrates the exponential convergence of spectral methods for smooth solutions.

Model Problem

Let us assume the differential equation:

$$-u''(x) = f(x), \quad x \in [-1, 1], \tag{4.31}$$

together with the boundary conditions:

$$u(-1) = 0, \quad u(1) = 0. \tag{4.32}$$

Chebyshev Collocation Method

Chebyshev Nodes The collocation nodes associated with chebyshev polynomials are defined as:

$$x_j = \cos\left(\frac{\pi j}{N}\right), \quad j = 0, 1, \ldots, N. \tag{4.33}$$

Approximation of the Solution We approximate the solution as:

$$u_N(x) = \sum_{k=0}^{N} a_k T_k(x), \tag{4.34}$$

where $T_k(x)$ denotes the Chebyshev polynomials.

Collocation Formulation The governing differential equation is imposed at the interior collocation points:

$$-u_N''(x_j) = f(x_j), \quad j = 1, \ldots, N-1. \tag{4.35}$$

Boundary conditions:

$$u_N(x_0) = 0, \quad u_N(x_N) = 0. \tag{4.36}$$

Spectral Differentiation Matrix

The first derivative is approximated as:

$$u'(x_i) \approx \sum_{j=0}^{N} D_{ij} u(x_j). \tag{4.37}$$

The second derivative is:

$$u''(x_i) \approx \sum_{j=0}^{N} (D^2)_{ij} u(x_j). \tag{4.38}$$

Thus, the governing equation becomes:

$$-(D^2\mathbf{u})_j = f(x_j). \tag{4.39}$$

Matrix Formulation

Let

$$\mathbf{u} = (u(x_0), u(x_1), \ldots, u(x_N))^T, \tag{4.40}$$

$$\mathbf{f} = (f(x_0), f(x_1), \ldots, f(x_N))^T. \tag{4.41}$$

Then the system becomes:

$$-D^2\mathbf{u} = \mathbf{f}. \tag{4.42}$$

After applying boundary conditions, we obtain:

$$A\mathbf{u} = \mathbf{b}. \tag{4.43}$$

Example with Exact Solution

Let

$$f(x) = \pi^2 \sin(\pi x). \tag{4.44}$$

For this problem,the exact analytical solution is:

$$u(x) = \sin(\pi x). \tag{4.45}$$

Procedure

1. Compute Chebyshev nodes x_j
2. Construct differentiation matrix D
3. Compute D^2
4. Evaluate $f(x_j)$
5. Solve the linear system
6. Compare with exact solution

Error Analysis

Define the maximum error:

$$E_N = \max_{0 \le j \le N} |u(x_j) - u_N(x_j)|. \tag{4.46}$$

Exponential Convergence

For smooth solutions, the error satisfies:

$$E_N \le Ce^{-\alpha N}. \tag{4.47}$$

Numerical Illustration

N	Error
10	10^{-5}
20	10^{-10}
30	10^{-14}

This demonstrates exponential decay of error.

Comparison with Other Methods

Method	Convergence Rate
Finite Difference	Algebraic $O(N^{-p})$
Finite Element	Polynomial
Spectral Method	Exponential

Advantages:

- Very high accuracy
- Fast convergence
- Efficient for smooth problems

Limitations:

- Gibbs phenomenon for discontinuities
- Dense matrices
- Difficult for complex domains

Chapter 5

Advanced Topics: Non-Classical Weights and Orthogonal Polynomials

5.1 Introduction

Orthogonal polynomials are widely used in fields such as approximation theory, computational mathematics, and spectral methods. Traditionally, these polynomials are studied using standard weight functions defined over fixed intervals. However, many real-world applications in science and engineering involve more complicated situations where the classical assumptions are no longer suitable. This has encouraged researchers to explore **non-classical weights** functions and **Sobolev orthogonal polynomials**, where the usual conditions on weights or inner products are modified.

In the case of **non-standard weights**, orthogonality may be defined with respect to measures that exhibit discontinuities (jumps) or internal singularities. Such weights arise naturally in problems involving heterogeneous media, boundary layers, or piecewise-defined physical properties. These irregularities significantly influence the structure of orthogonal polynomials, leading to modified recurrence relations and affecting convergence and approximation behavior.

An important generalization is provided by **Sobolev orthogonality**, where the inner product incorporates derivatives, typically of the form

$$\langle f, g \rangle = \int f(x)g(x)\,dx + \lambda \int f'(x)g'(x)\,dx,$$

reflecting not only function values but also their smoothness. This framework is particularly relevant in variational problems and partial differential equations, where solutions are naturally measured in energy norms.

These modern generalizations were developed to provide more accurate approximations for functions arising in complex applications. The resulting polynomial systems possess unique analytical and computational characteristics, making them an active and significant area of research in contemporary approximation theory.

5.2 Orthogonality with Respect to Non-Standard Weights

Let $w(x)$ be a real-valued weight function defined on an interval $I \subset \mathbb{R}$. A sequence of polynomials $\{P_n(x)\}$ is said to be orthogonal with respect to $w(x)$ if

$$\int_I P_n(x)P_m(x)w(x)\,dx = 0, \quad n \neq m.$$

In the non-classical setting, the weight function $w(x)$ may be discontinuous or unbounded.

5.3 Polynomials with a Weight Having a Jump Discontinuity

5.3.1 Jump Weight

Consider a weight function with a discontinuity at $c \in (a, b)$:

$$w(x) = \begin{cases} w_1(x), & x < c, \\ w_2(x), & x \geq c, \end{cases}$$

where $w_1(x)$ and $w_2(x)$ are positive functions.

5.3.2 Orthogonality Condition

The orthogonality condition becomes

$$\int_a^c P_n(x)P_m(x)w_1(x)\,dx + \int_c^b P_n(x)P_m(x)w_2(x)\,dx = 0, \quad n \neq m.$$

Properties

- The discontinuity at $x = c$ affects the structure of orthogonal polynomials.
- Zeros tend to cluster near the discontinuity.
- Recurrence relations may deviate from the classical three-term form.
- Approximation emphasizes regions where the weight is larger.

Example

Let

$$w(x) = \begin{cases} 1, & -1 \leq x < 0, \\ 2, & 0 \leq x \leq 1. \end{cases}$$

Then

$$\int_{-1}^0 P_n(x)P_m(x)\,dx + 2\int_0^1 P_n(x)P_m(x)\,dx = 0.$$

This shows that the interval $[0, 1]$ has greater influence on orthogonality.

5.4 Polynomials with Internal Singularities

Definition:

A weight function has an internal singularity if

$$w(x) = |x - c|^\alpha, \quad \alpha > -1, \quad c \in (a, b).$$

Types of Singularities:

- Weak singularity: $-1 < \alpha < 0$
- Vanishing weight: $\alpha > 0$

Orthogonality Relation:

$$\int_a^b P_n(x) P_m(x) |x - c|^\alpha \, dx = 0, \quad n \neq m.$$

Properties:

- The point $x = c$ strongly influences polynomial behavior.
- Zeros tend to cluster near the singularity.
- Convergence may slow near $x = c$.
- Standard uniform convergence may fail.

Example:

Consider

$$w(x) = |x|^\alpha, \quad x \in [-1, 1].$$

- If $\alpha > 0$, the weight vanishes at $x = 0$.
- If $-1 < \alpha < 0$, the weight becomes large near $x = 0$.

Thus, the polynomials either avoid or concentrate near the singular point depending on α.

Comparison Between Jump and Singular Weights

Feature	Jump Discontinuity	Singular Weight
Nature	Sudden change	Infinite/zero behavior
Zeros	Cluster near jump	Cluster near singularity
Smoothness	Piecewise smooth	Non-smooth
Approximation	Uneven accuracy	Localized distortion

5.5 Sobolev Orthogonal Polynomials

Introduction

In classical approximation theory, orthogonal polynomials are usually defined through an inner product of the form

$$\langle f, g \rangle = \int_a^b f(x) g(x) w(x) \, dx,$$

where $w(x)$ represents a weight function. However, in many applications, especially in numerical analysis and spectral methods, it is useful to include information about derivatives in the inner product. This leads to the concept of Sobolev orthogonality.

5.5.1 Sobolev Inner Product

A Sobolev inner product is a modified form of the standard inner product that includes both the functions and their derivatives.It is defined as:

$$\langle f, g\rangle_S = \int_a^b f(x)g(x)w_0(x)\,dx + \lambda \int_a^b f'(x)g'(x)w_1(x)\,dx,$$

where $w_0(x), w_1(x) \geq 0$ are weight functions and $\lambda > 0$.

A commonly used simplified form is

$$\langle f, g\rangle = \int f(x)g(x)\,dx + \lambda \int f'(x)g'(x)\,dx.$$

Definition

A sequence of polynomials $\{S_n(x)\}_{n=0}^{\infty}$ is called Sobolev orthogonal if

$$\langle S_n, S_m\rangle_S = 0 \quad \text{for } n \neq m.$$

Motivation

Sobolev orthogonal polynomials naturally appear in several mathematical and scientific applications,including:

- useful in advanced techniques for solving differential equations
- Smoothing and regularization problems
- Variational formulations in applied mathematics

Key Properties

- Orthogonality involves both function values and derivatives.
- These polynomials usually do not follow a simple three-term recurrence relation.
- Their behavior depends on the parameter λ.
- They provide smoother approximations.

5.5.2 Construction via Gram–Schmidt Process

Sobolev orthogonal polynomials can be generated using the Gram–Schmidt orthogonalization process applied to the basis $\{1, x, x^2, \dots\}$ with respect to the Sobolev inner product:

$$\langle f, g\rangle = \int fg + \lambda \int f'g'.$$

Example

Let us take the following inner product

$$\langle f, g \rangle = \int_0^1 f(x)g(x)\,dx + \lambda \int_0^1 f'(x)g'(x)\,dx.$$

First Polynomial

$$S_0(x) = 1$$

Second Polynomial

Let

$$S_1(x) = x - c.$$

Using orthogonality:

$$\langle S_1, S_0 \rangle = 0.$$

We compute:

$$\int_0^1 (x - c)\,dx + \lambda \int_0^1 (1)(0)\,dx = 0.$$

$$\frac{1}{2} - c = 0 \quad \Rightarrow \quad c = \frac{1}{2}.$$

Thus,

$$S_1(x) = x - \frac{1}{2}.$$

5.5.3 Comparison with Classical Orthogonal Polynomials

Feature	Classical OPs	Sobolev OPs
Inner Product	Function only	Function + derivatives
Recurrence Relation	Three-term	Generally absent
Smoothness	Moderate	Higher
Applications	Approximation	PDEs, spectral methods

Applications

- Spectral methods for solving differential equations
- Finite element methods
- Signal processing and smoothing
- Approximation theory with derivative constraints

Challenges and Research Directions

- Lack of explicit formulas in general cases
- Computational complexity
- Study of asymptotic behavior
- Extensions to higher-order derivatives and multidimensional cases

5.6 Modified Recurrence Relations and Altered Approximation Properties

In the traditional theory of orthogonal polynomials, the sequence $\{P_n(x)\}$ follows a three-term recurrence relation because of orthogonality with respect to a standard weight function $w(x)$ over an interval I. However, when non-classical weight functions or Sobolev-type inner products are introduced, the orthogonality structure changes considerably. Consequently, the recurrence relations, approximation properties, and convergence behavior are also modified.

Classical Recurrence Relation

Orthogonal polynomials satisfy the recurrence relation:

$$P_{n+1}(x) = (a_n x + b_n)P_n(x) - c_n P_{n-1}(x), \tag{5.1}$$

where a_n, b_n, c_n are real constants determined by the weight function.

Sobolev Inner Product

A Sobolev-type inner product can be written as:

$$\langle f, g\rangle_S = \int_I f(x)g(x)w(x)\,dx + \lambda \int_I f'(x)g'(x)v(x)\,dx, \tag{5.2}$$

where $\lambda > 0$ and $w(x), v(x)$ are weight functions.

5.6.1 Modified Recurrence Relations

Non-Classical Weights

When the weight function is non-standard (for example, having jump discontinuities or internal singularities), the orthogonality measure is no longer smooth. This leads to:

- Irregular behavior of recurrence coefficients a_n and b_n
- Loss of symmetry
- Possibility of higher-term recurrence relations

In such cases, multiplication by x does not necessarily project onto only two neighboring polynomials.

Sobolev Orthogonal Polynomials

For Sobolev orthogonality, the inner product is expressed as:

$$\langle f, g\rangle = \int f(x)g(x)w(x)\,dx + \lambda \int f'(x)g'(x)w_1(x)\,dx, \tag{5.3}$$

where $\lambda > 0$.

This introduces derivative terms, fundamentally altering the orthogonality structure. As a result:

- The classical three-term recurrence relation generally fails
- Higher-order recurrence relations arise
- Recurrence relations may involve derivatives or matrix formulations

A generalized recurrence may take the form:

$$P_{n+1}(x) = (x - a_n)P_n(x) - b_n P_{n-1}(x) + \sum_{k=0}^{m} c_{n,k} P_k(x). \tag{5.4}$$

5.6.2 Altered Approximation Properties

Classical Approximation

In the classical case:

- Approximation is optimal in the L^2 norm
- Convergence depends on smoothness
- Error is minimized in the mean-square sense

Effects of Non-Classical Weights

For irregular weights:

- Approximation deteriorates near singularities
- Non-uniform convergence occurs
- Gibbs-type oscillations may appear

Sobolev Approximation

Sobolev orthogonality introduces the norm:

$$\|f\|_S^2 = \int |f(x)|^2 dx + \lambda \int |f'(x)|^2 dx. \tag{5.5}$$

Key implications include:

- Improved smoothness of approximations
- Better approximation of derivatives
- Enhanced convergence for smooth functions

Comparison with Classical Approximation

Feature	Classical Case	Sobolev Case
Norm	L^2	Sobolev norm
Recurrence	Three-term	Multi-term
Smoothness	Not enforced	Enforced
Derivative control	Weak	Strong
Applications	Interpolation	PDEs, Variational problems

5.6.3 Motivation for Generalizations

1. Physical and Engineering Applications

Many real-world systems involve discontinuities or singularities. Classical orthogonal polynomials are insufficient in such cases, motivating the use of generalized orthogonality.

2. Variational Problems

In problems involving energy minimization:

$$E[f] = \int |f'(x)|^2 dx, \tag{5.6}$$

Sobolev norms arise naturally. Sobolev orthogonal polynomials serve as optimal basis functions in such settings.

3. Numerical Methods

Sobolev orthogonality plays a key role in:

- Finite Element Methods (FEM)
- Spectral methods for partial differential equations

4. Stability and Regularization

Including derivative terms:

- Reduces oscillations
- Improves numerical stability
- Acts as a regularization mechanism

5.7 Approximation in Variational Problems Using Energy Norms

5.7.1 Variational Principles

Many problems can be formulated as minimizing an energy functional:

$$J[u] = \int_I \left(|u'(x)|^2 + |u(x)|^2\right) dx. \tag{5.7}$$

5.7.2 Energy Norm

The related energy norm can be expressed as:

$$\|u\|_E^2 = \int_I \left(|u'(x)|^2 + |u(x)|^2\right) dx. \tag{5.8}$$

5.7.3 Approximation Strategy

We approximate the solution as:

$$u_n(x) = \sum_{k=0}^{n} c_k S_k(x), \tag{5.9}$$

where $\{S_k(x)\}$ denotes the Sobolev orthogonal polynomials.

5.7.4 Galerkin Method

The coefficients are determined by:

$$\langle u - u_n, S_k \rangle_S = 0. \tag{5.10}$$

5.7.5 Example: Boundary Value Problem

Consider:

$$-u''(x) + u(x) = f(x), \quad x \in [a, b]. \tag{5.11}$$

The weak formulation is:

$$\int_a^b (u'v' + uv)\, dx = \int_a^b f(x)v(x)\, dx. \tag{5.12}$$

5.7.6 Approximation Using Sobolev Polynomials

Substituting the approximation:

$$\sum_{k=0}^{n} c_k \langle S_k, S_j \rangle_S = \langle f, S_j \rangle. \tag{5.13}$$

This yields a linear system for the coefficients c_k.

Advantages

- Minimizes the energy functional directly.
- Handles derivative constraints effectively.
- Provides stable numerical approximations.
- Suitable for spectral methods.

Physical Interpretation

The derivative term represents energy (e.g., strain energy in mechanics). Minimizing the Sobolev norm corresponds to finding the minimum energy configuration of the system.

Convergence

If $u \in H^k(I)$, then:

$$\|u - u_n\|_S \to 0 \quad \text{as } n \to \infty. \tag{5.14}$$

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