VSB TECHNICAL UNIVERSITY OF OSTRAVA | FACULTY OF ELECTRICAL ENGINEERING AND COMPUTER SCIENCE

Approximation of Karhunen-Loève Decomposition of Isotropic Gaussian Random Fields Using Orthogonal Polynomials and Gaussian Quadratures

Aproximace Karhunen-Loèveho rozkladu izotropních Gaussovských náhodných polí pomocí ortogonálních polynomů a Gaussových kvadratur

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Bachelor Thesis

Supervisor: Ing. Michal Béreš, Ph.D.

Ostrava, 2025

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Ref. no.VSB/24/139087
vsboee2403F8C1

Bachelor Thesis Assignment

Student: **Michal Sedlář**

Study Programme: B0541A170008 Computational and Applied Mathematics

Title: Approximation of Karhunen-Loève Decomposition of Isotropic Gaussian Random Fields Using Orthogonal Polynomials and Gaussian Quadratures
Aproximace Karhunen-Loèveho rozkladu izotropních Gaussovských náhodných polí pomocí ortogonálních polynomů a Gaussových kvadratur

The thesis language: English

Description:

The goal of this thesis is to utilize orthogonal polynomials and Gaussian quadratures for the efficient approximation of the Karhunen-Loève decomposition of isotropic Gaussian random fields.

In the theoretical part, the student will familiarize themselves with the basic theory of orthogonal polynomials, including their evaluation using recursive formulas. The focus will then shift to the computation of Gaussian quadrature points and weights using the Golub-Welsch algorithm. The final part of the theoretical work is dedicated to the Karhunen-Loève decomposition of isotropic Gaussian random fields.

In the practical part, the student will concentrate on the implementation of the mentioned methods and their use in approximating the Karhunen-Loève decomposition.

References:

T.S. Chihara. (1978). An Introduction to Orthogonal Polynomials (Gordon and Breach, New York)
Gautschi, Walter. (2004). Orthogonal polynomials: computation and approximation. OUP Oxford.
Golub, G. H., & Welsch, J. H. (1969). Calculation of Gauss quadrature rules. Mathematics of computation, 23(106), 221-230.
Lord, G. J., Powell, C. E., & Shardlow, T. (2014). An Introduction to Computational Stochastic PDEs (Vol. 50). Cambridge University Press.

Extent and terms of a thesis are specified in directions for its elaboration that are opened to the public on the web sites of the faculty.

Supervisor: **Ing. Michal Béreš, Ph.D.**

Date of issue: 01.09.2024

Date of submission: 30.04.2025

Study programme guarantor: prof. RNDr. Jiří Bouchala, Ph.D.

In IS EDISON assigned: 22.11.2024 12:08:55

Abstrakt

Cílem této práce je definovat a naimplementovat efektivní způsob pro aproximaci Karhunen-Loèveho rozkladu. Práce nejprve poskytuje přehled teorie týkající se ortogonálních polynomů, vážených skalárních součinů a Gaussových kvadraturních pravidel. Klíčové myšlenky jsou vysvětleny jasným a přístupným způsobem. Mezi ně patří tříčlenný rekurentní vztah pro generování ortogonálních polynomů a Golubův-Welschův algoritmus pro výpočet kvadraturních uzlů a vah z přidružené Jacobiho matice. Jsou představeny základní koncepty z teorie pravděpodobnosti se zaměřením na kovarianční funkce a Gaussovská náhodná pole, aby byl vytvořen nezbytný základ pro hlavní aplikaci zkoumanou v této práci. Hlavní aplikace ukazuje použití Galerkinovy metody, společně s bázemi ortogonálních polynomů a Gaussovými kvadraturními pravidly, k dosažení efektivní numerické aproximace Karhunen-Loèveho (KL) rozkladu pro stochastické procesy. Všechny diskutované metody jsou implementovány v jazyce Python a odpovídající kód je dostupný v uvedeném repozitáři [1].

Klíčová slova

Legendrovy polynomy, Gaussova kvadratura, Galerkinova metoda, Karhunen-Loèveho rozklad, tříčlenná rekurze, Jacobiho matice

Abstract

The goal of this thesis is to define and implement an efficient method to approximate the Karhunen-Loève decomposition. The thesis first provides a review of the theory related to orthogonal polynomials, weighted inner products, and Gaussian quadrature rules. Key ideas are explained in a clear and accessible way. These include the three-term recurrence relation for generating orthogonal polynomials and the Golub-Welsch algorithm for computing quadrature nodes and weights from the associated Jacobi matrix. Fundamental concepts from probability theory are introduced, focusing on covariance functions and Gaussian random fields, to establish the necessary background for the primary application explored in this work. The core application demonstrates the use of the Galerkin method, together with orthogonal polynomial bases and Gaussian quadrature rules, to achieve an efficient numerical approximation of the Karhunen-Loève (KL) expansion for stochastic processes. All methods discussed are implemented in Python, and the corresponding code is available at the specified repository [1].

Keywords

Legendre polynomials, Gauss quadrature rule, Galerkin method, Karhunen-Loève expantion, three-term recurrence, Jacobi matrix

Acknowledgement

I would like to thank Ing. Michal Béreš, Phd. for his guidance and help with the thesis and my family for supporting me in my studies.

Contents

List of symbols and abbreviations

$\mathbb{R}$	–	The set of real numbers
$\mathbb{R}^n$	–	n-dimensional Euclidean space
$\mathbb{R}_0^+$	–	The set of non-negative real numbers ($\langle 0, \infty\rangle$)
$\mathbb{N}$	–	The set of natural numbers $\{1, 2, 3, \dots\}$
$\mathbb{N}_0$	–	The set of natural numbers including zero $\{0, 1, 2, \dots\}$
I	–	A finite interval $\langle a, b\rangle \subset \mathbb{R}$
$\mathcal{T}$	–	Domain of a random field (a subset of $\mathbb{R}^d$)
P	–	The space of all real polynomials
P_d	–	The space of real polynomials of degree at most d
P_d^m	–	The set of monic polynomials of degree exactly d
$\widetilde{P_d}$	–	The set of normalized polynomials of degree d
$C(I)$	–	The space of continuous functions on the interval I
$L^2(I)$	–	Hilbert space of square-integrable functions on the interval I
V_N, V_N^x, V_M^y	–	Finite-dimensional function subspaces
$V_N^x \otimes V_M^y$	–	Tensor product space
Ω	–	Sample space
$\mathcal{F}, \mathit{\Sigma}$	–	Sigma-algebra on Ω
$w(x)$	–	Weight function
$\langle \cdot, \cdot \rangle_w$	–	Weighted inner product with weight $w(x)$
$\Vert\cdot\Vert_w$	–	Norm derived from the weighted inner product $\langle \cdot, \cdot \rangle_w$
$\Vert\cdot\Vert_{L^2}$	–	L^2-norm over a specified interval
$\langle \cdot, \cdot \rangle_{L^2}$	–	L^2-inner product over a specified interval
$\pi_k(x)$	–	Monic orthogonal polynomial of degree k
$\tilde{\pi}_k(x)$	–	Orthonormal polynomial of degree k
$\pi_k^L(x)$	–	Monic Legendre polynomial of degree k
$\tilde{\pi}_k^L(x)$	–	Orthonormal Legendre polynomial of degree k
$\mathbb{P}$	–	Probability measure
$X, Y, X(t), u(\boldsymbol{x})$	–	Random variables, stochastic processes, random fields

$\mathbb{E}[\cdot]$	–	Expected value operator
$\mathrm{Cov}(\cdot,\cdot)$	–	Covariance operator between two random variables
$C(s,t), c(\boldsymbol{x},\boldsymbol{y})$	–	Autocovariance function of a process/field
$c(\tau)$	–	Stationary covariance function (1D)
$c^0(r)$	–	Isotropic covariance function
$N(\mu,\sigma^2)$	–	Gaussian (normal) distribution with mean μ and variance σ^2
$\mathrm{span}\{\cdot\}$	–	Span of a set of vectors or functions
α_k, β_k	–	Coefficients in the three-term recurrence relation
λ_j	–	Eigenvalue of covariance operator or Quadrature weight (context-dependent)
u_j	–	Eigenfunction of covariance operator
τ_j	–	Quadrature node (root of orthogonal polynomial)
σ^2	–	Variance
$\delta_{k,0}, \delta_{kj}$	–	Kronecker delta
$\boldsymbol{x}, \boldsymbol{y}$	–	Vectors in $\mathbb{R}^d$
$\tilde{\boldsymbol{\pi}}(x)$	–	Vector of orthonormal polynomials $[\tilde{\pi}_0(x),\ldots,\tilde{\pi}_{n-1}(x)]^T$
$\boldsymbol{\tau}^{(n)}$	–	Vector of roots $[\tau_0^{(n)},\ldots,\tau_{n-1}^{(n)}]^T$
$\boldsymbol{e}_n$	–	n-th standard basis vector $[0,\ldots,0,1]^T$
$\boldsymbol{\lambda}^G$	–	Vector of Gauss weights $[\lambda_1^G,\ldots,\lambda_n^G]^T$
$\boldsymbol{e}$	–	Vector of ones $[1,1,\ldots,1]^T$
J_n	–	$n \times n$ Jacobi matrix

PDF	–	probability density function
GRF	–	Gaussian Random Field
KL	–	Karhunen-Loève

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Chapter 1

Introduction

In many areas of science and engineering, we encounter systems or phenomena that involve randomness or uncertainty. Instead of having fixed values, measurements might vary unpredictably. Mathematical objects called stochastic processes, or more generally random fields (as introduced in Chapter 3), are used to model such situations where values change randomly over time or space. Examples include variations in material properties or fluctuating forces acting on a structure. However, random fields can possess infinite complexity, therefore working directly with them can be very difficult. A powerful technique to simplify them is the Karhunen-Loève (KL) expansion [2, 3], which is a central topic of this thesis (discussed in Chapter 4). The KL expansion represents a random field as a sum of specific, deterministic functions multiplied by random coefficients. These deterministic functions capture the main spatial patterns of the randomness, and the random coefficients capture the uncertainty in the magnitude of these patterns. A key property is that these random coefficients are uncorrelated (and for Gaussian fields, independent), which simplifies analysis. The KL expansion is considered optimal because it captures the most variance (randomness) of the field using the fewest terms in the sum, making it efficient for representing complex random behavior in a manageable way.

The core of finding the KL expansion involves solving a specific mathematical problem: finding the eigenfunctions u_j and eigenvalues λ_j of an integral operator defined by the random field's autocovariance function $c(\boldsymbol{x}, \boldsymbol{y})$. This function describes how related the random values are at different points $\boldsymbol{x}$ and $\boldsymbol{y}$. The problem we need to solve looks like this:

$$\int_{\mathcal{T}} c(\boldsymbol{x}, \boldsymbol{y}) u_j(\boldsymbol{y}) d\boldsymbol{y} = \lambda_j u_j(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathcal{T}. \tag{1.1}$$

This is known as an integral eigenvalue problem. Finding exact analytical solutions (u_j and λ_j) is usually impossible except in very simple cases. Therefore, we need numerical methods to find approximate solutions.

This thesis focuses on a practical numerical approach to compute the approximate KL expansion. The chosen method is the Galerkin method (detailed in Chapter 4). The Galerkin method transforms the difficult integral eigenvalue problem into a more standard matrix eigenvalue problem, which can be solved using computational linear algebra techniques.

To use the Galerkin method effectively, we need two key ingredients developed in the earlier parts of this thesis:

1. **Basis Functions:** The Galerkin method approximates the unknown eigenfunctions u_j as combinations of known, simpler functions called basis functions. A good choice for these basis functions, especially when working on intervals, are orthogonal polynomials. Chapter 2 introduces orthogonal polynomials, focusing on Legendre polynomials. It explains how they are constructed using recurrence relations and how they relate to Jacobi matrices. We also see how to adapt them for any finite interval $\langle a, b \rangle$. Using an orthonormal basis simplifies the Galerkin formulation.

2. **Numerical Integration:** Setting up the matrix eigenvalue problem in the Galerkin method requires calculating several integrals involving the basis functions and the covariance function $c(\boldsymbol{x}, \boldsymbol{y})$. Calculating these integrals accurately and efficiently is crucial. Gaussian quadrature is a very effective technique for numerical integration, especially when integrating polynomials or functions well-approximated by polynomials. Chapter 2 also details Gaussian quadrature, showing how the necessary quadrature nodes (τ_j) and weights (ω_j) can be computed directly from the Jacobi matrix associated with the orthogonal polynomials using the Golub-Welsch algorithm [4]. The efficiency and accuracy of this quadrature method are demonstrated in the numerical experiments at the end of Chapter 2.

Therefore, this thesis builds a computational pipeline: We use the theory of orthogonal polynomials (Chapter 2) to generate basis functions (Legendre polynomials) and to construct efficient Gaussian quadrature rules (via Jacobi matrices and Golub-Welsch). We then use these tools within the Galerkin method (Chapter 4) to approximate the solution of the integral eigenvalue problem (1.1) arising from the autocovariance function (introduced in Chapter 3). The result is a numerical approximation of the Karhunen-Loève expansion for a given random field (see [1]).

The structure of this thesis follows this logical progression:

- Chapter 2: Provides the mathematical foundation related to orthogonal polynomials. Key topics include weighted inner products, the three-term recurrence relation, Jacobi matrices, Gaussian quadrature rules, the Golub-Welsch algorithm for computing nodes and weights, and the generalization of Legendre polynomials to arbitrary finite intervals. The end of this chapter demonstrates the concepts through numerical examples. This includes generating polynomials, timing the quadrature rule computation, and testing the convergence of Gaussian quadrature for integrating different types of functions.

- Chapter 3: Introduces the necessary concepts from probability theory to understand random fields. This covers L^2 space, basic probability definitions, random variables, stochastic processes, random fields, expectation, covariance, autocovariance functions, and Gaussian random fields (GRF).
- Chapter 4: Focuses on the Karhunen-Loève expansion itself. It presents the KL theorem and explains how to approximate the required eigenvalues and eigenfunctions using the Galerkin method with orthogonal polynomial basis functions. The role of Gaussian quadrature in computing the resulting integrals is emphasized. Numerical experiments show the computed KL components and their accuracy.
- Chapter 5: Briefly summarizes the work presented and the results obtained.

By following these steps, this thesis aims to provide a clear description and practical implementation of methods used to compute the Karhunen-Loève expansion, relying heavily on the properties of orthogonal polynomials and associated numerical techniques.

Chapter 2

Polynomials

This section is devoted to introduction of orthogonal polynomials with respect to given inner products. The inner products considered throughout this work are defined via integration over a specified interval I with respect to a continuous weight function $w \in C(I)$. A key characteristic of orthogonal polynomials with respect to these inner products, and by extension their normalized counterparts (orthonormal polynomials), is that they satisfy a three-term recurrence relation. The coefficients of this recurrence relation can be arranged into a symmetric tridiagonal matrix, known as the Jacobi matrix. The eigenpairs of this Jacobi matrix provide a direct method for determining the roots of the orthogonal polynomials. The chapter concludes with a discussion on Gaussian quadrature rules, which utilize the roots of orthogonal polynomials as nodes and derived values as weights for numerical integration. The eigenvalue (spectral) decomposition of the aforementioned Jacobi matrix yields, via Golub-Welsch algorithm [4], these quadrature nodes and weights. For Legendre polynomials, we also show how to extend them over a finite interval with the use of a simple affine transformation of variables.

The section is organized as follows. Section 2.1 introduces monic polynomials. Section 2.2 defines the weighted inner product and the orthonormal basis. Section 2.3 presents the definition of Jacobi matrix derived from the three-term recurrence. Section 2.4 introduces the quadrature rule for approximating integrals over finite intervals. Section 2.5 describes the Golub-Welsch algorithm for computing quadrature nodes and weights. Section 2.6 focuses on Legendre polynomials and their affine generalizations.

Standard results from linear algebra and functional analysis are used freely; key references for orthogonal polynomials are [5, 6, 7].

2.1 Polynomials of real variable

The scope of this study is confined to polynomials with real coefficients and of a real variable. A polynomial is considered as monic if its leading coefficient is equal to one. Specifically, a polynomial $p(x) = a_n x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0$ of degree n is monic if $a_n = 1$.

Definition 1 (Space of Polynomials)**.** For a non-negative integer d, let us define

$$P_d \coloneqq \left\{ p(x) = \sum_{i=0}^{d} a_i x^i \;\middle|\; a_i \in \mathbb{R} \right\}$$

as the space of real polynomials of degree at most d. The space of all real polynomials is then

$$P \coloneqq \bigcup_{d=0}^{\infty} P_d.$$

Definition 2 (Monic polynomials)**.** For a non-negative integer d, let us define

$$P_d^m \coloneqq \left\{ \pi(x) = x^d + \sum_{i=0}^{d-1} a_i x^i \;\middle|\; a_i \in \mathbb{R} \right\}$$

as the set of *monic polynomials* of degree exactly d.

2.2 Weighted Inner product

In this thesis we constraint ourselves to continuous weight functions, instead of the more general approach considering general measures as in [5]. To define a weighted inner product properly, we first define a strictly positive continuous weight function $w(x)$ on a closed interval and the related symmetric bilinear form, denoted $\langle \cdot, \cdot \rangle_w$. It is demonstrated that this form is positive definite, i.e., it is a weighted inner product. For clarity and conciseness in the subsequent parts, the primary focus will be restricted to the specific case defined over the interval $I = \langle -1, 1 \rangle$ with the unity weight function $w(x) = 1$.

Definition 3 (Weight Function)**.** Let $I = \langle a, b \rangle \subset \mathbb{R}, b > a$ (a bounded, closed interval). A function $w(x) \in C(I)$ that satisfies

$$\forall x \in I : w(x) > 0,$$

is called a *weight function.*

Remark 4. The weighted integral is well defined for all $f \in C(I)$:

$$\int_I f(x)w(x)\,dx \in \mathbb{R}.$$

Theorem 5 (Moments of a Weight Function)**.** *Let $w(x), I$ be a weight function and corresponding support. Then all moments are finite:*

$$\mu_r := \int\limits_I x^r w(x)\, dx \in \mathbb{R},\ r = 0, 1, 2, \ldots .$$

Definition 6 (Weighted bilinear form)**.** For a weight function $w(x)$ and its corresponding support I, we define the symmetric bilinear form $\langle \cdot, \cdot \rangle_w$ for all $u, v \in C(I)$ as:

$$\langle u, v \rangle_w = \int\limits_I u(x)v(x)w(x)\, dx.$$

Definition 7. The operator $\|u\|_w : C\left(I\right) \to \mathbb{R}_0^+$, derived from the bilinear form $\langle \cdot, \cdot \rangle_w$, is defined as

$$\|u\|_w = \sqrt{\langle u, u \rangle_w}.$$

Definition 8 (Positive definiteness)**.** A bilinear form $\langle \cdot, \cdot \rangle_w$ on $C\left(I\right)$ is said to be positive definite if

$$\|u\|_w > 0, \quad \forall u \in C\left(I\right) : u \not\equiv 0.$$

Lemma 9 (Inner product over $\langle -1, 1 \rangle$)**.** *A symmetric bilinear form $\langle \cdot, \cdot \rangle_w$ with the weight function $w(x) = 1$ and corresponding support $I = \langle -1, 1 \rangle$*

$$\langle u, v \rangle_w = \int\limits_{-1}^{1} u(x)v(x)\, dx$$

is positive definite on $C\left(I\right)$, i.e. it is an inner product.

Proof. Let $u \in C\left(\langle -1, 1 \rangle\right)$ be a nonzero function, that is, $u \not\equiv 0$. Then, there exists some point $x_0 \in \langle -1, 1 \rangle$ such that $u(x_0) \neq 0$. Without loss of generality, assume $u(x_0) > 0$ (if $u(x_0) < 0$, consider $-u$ instead). Let

$$\varepsilon = \frac{u(x_0)}{2} > 0.$$

Since u is continuous, for this ε, there exists a $\delta > 0$ such that for all x in the interval $I_\delta = (x_0 - \delta, x_0 + \delta) \cap \langle -1, 1 \rangle$, we have:

$$|u(x) - u(x_0)| < \varepsilon.$$

Note that I_δ has positive length $|I_\delta| \geq \min\left(\delta, 1\right) > 0$. Then, for every $x \in I_\delta$, it follows that

$$u(x) > u(x_0) - \varepsilon = \frac{u(x_0)}{2} > 0.$$

This implies that

$$u(x)^2 > \left(\frac{u(x_0)}{2}\right)^2 .$$

Integrating both sides over the interval I_δ, we get:

$$\int\limits_{I_\delta} u(x)^2\,dx \geq \int\limits_{I_\delta} \left(\frac{u(x_0)}{2}\right)^2 dx = \left(\frac{u(x_0)}{2}\right)^2 \cdot |I_\delta| \,,$$

The squared norm $\|u\|_w^2$ satisfies

$$\|u\|_w^2 = \int\limits_I u(x)^2\,dx \geq \int\limits_{I_\delta} u(x)^2\,dx,$$

therefore

$$\|u\|_w^2 \geq \left(\frac{u(x_0)}{2}\right)^2 \cdot |I_\delta| > 0.$$

This shows that $\|u\|_w > 0$ for every nonzero function $u \in C\left(\langle -1, 1\rangle\right)$, and so the inner product is positive definite on $C\left(\langle -1, 1\rangle\right)$. □

Corollary 10 (to Lemma 9)**.** *Bilinear form $\langle \cdot, \cdot \rangle_w$ is an inner product for all $w(x)$ from Definition 3 and $\|\cdot\|_w$* is *a* norm on $C\left(I\right)$.

Remark 11. If $\langle u, v\rangle_w = 0$, then u and v are said to be *orthogonal* with respect to the inner product $\langle \cdot, \cdot \rangle_w$.

Theorem 12 (Shift Property)**.** *The inner product $\langle \cdot, \cdot \rangle_w$ has the property:*

$$\langle xu, v\rangle_w = \langle u, xv\rangle_w \,, \quad \forall u, v \in P_d \quad \forall x \in \mathbb{R}.$$

i.e., we say it has the shift property*.*

Proof. The shift property holds for an inner product defined by weighted integrals:

$$\langle xu, v\rangle_w = \int\limits_I \left(xu(x)\right) v(x) w(x)\,dx = \int\limits_I u(x) \left(xv(x)\right) w(x)\,dx = \langle u, xv\rangle_w \,.$$

□

Definition 13 (Normalized polynomials)**.** For a non-negative integer d, the set of normalized polynomials with respect to the inner product $\langle \cdot, \cdot \rangle_w$ and norm $\|\cdot\|_w$ is defined as

$$\widetilde{P_d} \coloneqq \left\{\tilde{p} \in P_d : \|\tilde{p}\|_w = 1\right\}.$$

Given the definition of the weighted inner product $\langle \cdot, \cdot \rangle_w$, a key objective is the construction of a corresponding sequence of orthogonal polynomials. A fundamental theorem guarantees that for such inner product defined on the space of polynomials, there exists an infinite sequence $\{\pi_k(x)\}_{k=0}^{\infty}$ of polynomials such that $\langle \pi_j, \pi_k \rangle_w = 0$ for $j \neq k$. Furthermore, this sequence can be uniquely determined by imposing the additional constraint that each polynomial $\pi_k(x)$ is monic.

Theorem 14 ([5, Theorem 1.6])**.** *Let $\langle \cdot, \cdot \rangle_w$ be inner product on P, then there exists a unique infinite sequence $\{\pi_k\}_{k=0}^{\infty}$ of monic orthogonal polynomials.*

2.3 Three-term recurrence

For any inner product $\langle \cdot, \cdot \rangle_w$, there exists a basis $\{\pi_k\}_{k=0}^{\infty}$ for the polynomial space consisting of mutually orthogonal polynomials. Leveraging the properties of integral inner product, specifically the shift property, allows for the derivation of the three-term recurrence relation for these orthogonal polynomials. The coefficients of this recurrence relation also form a symmetric tridiagonal matrix, commonly referred to as the Jacobi matrix associated with the polynomial sequence. Crucially, the spectral decomposition of Jacobi matrix J_n provides essential information: its eigenvalues correspond precisely to the roots of the n-th orthogonal (and orthonormal) polynomial, and its eigenvectors are the previous orthonormal polynomials evaluated at these roots.

Theorem 15 (Three-term recurrence [5, Theorem 1.27])**.** *Let $\pi_k, k = 0, 1, 2, \ldots,$ be monic orthogonal polynomials with respect to the inner product $\langle \cdot, \cdot \rangle_w$. Then,*

$$\pi_{k+1}(x) = (x - \alpha_k)\,\pi_k(x) - \beta_k \pi_{k-1}(x), \quad k = 0, 1, 2, \ldots,$$

$$\pi_{-1}(x) = 0, \pi_0(x) = 1,$$

where

$$\alpha_k = \frac{\langle x\pi_k, \pi_k \rangle_w}{\langle \pi_k, \pi_k \rangle_w}, \quad k = 0, 1, 2, \ldots,$$

$$\beta_k = \frac{\langle \pi_k, \pi_k \rangle_w}{\langle \pi_{k-1}, \pi_{k-1} \rangle_w}, \quad k = 1, 2, \ldots,$$

$$\beta_0 = \langle \pi_0, \pi_0 \rangle_w .$$

Proof. We are going to generate a sequence of orthogonal polynomials $\{\pi_k(x)\}$ using a Gram-

Schmidt process:

$$\begin{aligned}\pi_0(x) &= f_0(x)\\ \pi_1(x) &= f_1(x) - \frac{\langle f_1, \pi_0\rangle_w}{\langle \pi_0, \pi_0\rangle_w}\pi_0(x)\\ &\vdots\\ \pi_k(x) &= f_k(x) - \sum_{i=1}^{k-1}\frac{\langle f_k, \pi_i\rangle_w}{\langle \pi_i, \pi_i\rangle_w}\pi_i(x);\end{aligned}$$

with $f_0(x) = 1$ and each subsequent function to be orthogonalized is constructed as $f_{k+1}(x) = x\pi_k(x)$. Note that by this construction, π_k are monic and orthogonal polynomials. In the $(k+1)$-th step, $f_{k+1}(x)$ is orthogonalized against the subspace spanned by $\{\pi_0, \dots, \pi_k\}$. The polynomial $\pi_{k+1}(x)$ can then be represented as

$$\pi_{k+1}(x) = x\pi_k(x) - \sum_{i=1}^{k}\frac{\langle x\pi_k, \pi_i\rangle_w}{\langle \pi_i, \pi_i\rangle_w}\pi_i(x).$$

Expanding the sum, we have

$$\pi_{k+1}(x) = x\pi_k(x) - \frac{\langle x\pi_k, \pi_k\rangle_w}{\langle \pi_k, \pi_k\rangle_w}\pi_k(x) - \frac{\langle x\pi_k, \pi_{k-1}\rangle_w}{\langle \pi_{k-1}, \pi_{k-1}\rangle_w}\pi_{k-1}(x) - \sum_{i=0}^{k-2}\frac{\langle x\pi_k, \pi_i\rangle_w}{\langle \pi_i, \pi_i\rangle_w}\pi_i(x). \tag{2.1}$$

By the shift property of the inner product, we have

$$\forall k, i \in \mathbb{N} : \langle x\pi_k, \pi_i\rangle_w = \langle \pi_k, x\pi_i\rangle_w .$$

Since $x\pi_i$ is a polynomial of degree $i+1$, i.e. $x\pi_i \in P_{i+1}$, we can express $x\pi_i$ as a linear combination of the orthogonal polynomials up to degree $i+1$:

$$x\pi_i(x) = \sum_{j=0}^{i+1} c_j\pi_j(x), \tag{2.2}$$

for certain constants c_j. Then, for $k > i+1$, $\langle \pi_k, x\pi_i\rangle_w$ is zero due to the orthogonality of the polynomials:

$$\langle x\pi_k, \pi_i\rangle_w = \langle \pi_k, x\pi_i\rangle_w = \sum_{j=0}^{i+1} c_j \langle \pi_k, \pi_j\rangle_w = 0, \quad \forall k > i+1.$$

This leads to the simplification of (2.1) as

$$\pi_{k+1}(x) = x\pi_k(x) - \frac{\langle x\pi_k, \pi_k\rangle_w}{\langle \pi_k, \pi_k\rangle_w}\pi_k(x) - \frac{\langle x\pi_k, \pi_{k-1}\rangle_w}{\langle \pi_{k-1}, \pi_{k-1}\rangle_w}\pi_{k-1}(x),$$

which simplifies further to

$$\pi_{k+1}(x) = \left(x - \frac{\langle x\pi_k, \pi_k \rangle_w}{\langle \pi_k, \pi_k \rangle_w} \right) \pi_k(x) - \frac{\langle \pi_k, \pi_k \rangle_w}{\langle \pi_{k-1}, \pi_{k-1} \rangle_w} \pi_{k-1}(x).$$

Which yields $\alpha_k = \frac{\langle x\pi_k, \pi_k \rangle_w}{\langle \pi_k, \pi_k \rangle_w}$ for all $k = 0, 1, \ldots$, $\beta_0 = \langle \pi_0, \pi_0 \rangle_w$, and $\beta_k = \frac{\langle \pi_k, \pi_k \rangle_w}{\langle \pi_{k-1}, \pi_{k-1} \rangle_w}$ for all $k = 1, 2, \ldots$, i.e. we obtain the desired three-term recurrence relation:

$$\pi_{k+1}(x) = (x - \alpha_k)\, \pi_k(x) - \beta_k \pi_{k-1}(x).$$

□

Remark 16. Legendre polynomials $\pi_k^L(x)$ are orthogonal polynomials with respect to the standard inner product (weight $w(x) = 1$) over the interval $I^L = \langle -1, 1 \rangle$. The coefficients α_k and β_k for the three-term recurrence relation (Theorem 15) for these monic orthogonal polynomials are given by $\beta_0 = 2$; $\alpha_k = 0$ for $k = 0, 1, \ldots$; and $\beta_k = 1/(4 - k^{-2})$ for $k = 1, 2, \ldots$ (see [5, Table 1.1]).

Having a series of orthogonal polynomials and induced norm $\|\cdot\|_w$, we can form the orthonormal basis. Orthonormal basis can also be represented via three-term recurrence, tied to recurrence for monic orthogonal polynomials.

Theorem 17 ([5, Theorem 1.29])**.** *Let $\tilde{\pi}_k$, $k = 0, 1, 2, \ldots,$ be a series of orthonormal polynomials. Then,*

$$\sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(x) = (x - \alpha_k)\, \tilde{\pi}_k(x) - \sqrt{\beta_k}\tilde{\pi}_{k-1}(x), \quad k = 0, 1, 2, \ldots,$$
$$\tilde{\pi}_{-1}(x) = 0, \quad \tilde{\pi}_0(x) = 1/\sqrt{\beta_0},$$

where α_k, β_k, and β_0 are defined in Theorem 15.

Proof. Monic orthogonal polynomials π_k relate to the corresponding orthonormal polynomials $\tilde{\pi}_k$ via $\pi_k = \tilde{\pi}_k \|\pi_k\|_w$, where $\|\pi_k\|_w = \sqrt{\langle \pi_k, \pi_k \rangle_w}$ for all $k \in \mathbb{N}_0$. Therefore, the three-term recurrence from Theorem 15 can be rewritten as:

$$\tilde{\pi}_{k+1}\sqrt{\langle \pi_{k+1}, \pi_{k+1} \rangle_w} \;=\; (x - \alpha_k)\, \tilde{\pi}_k \sqrt{\langle \pi_k, \pi_k \rangle_w} - \beta_k \tilde{\pi}_{k-1} \sqrt{\langle \pi_{k-1}, \pi_{k-1} \rangle_w}$$

$$\tilde{\pi}_{k+1}\sqrt{\frac{\langle \pi_{k+1}, \pi_{k+1} \rangle_w}{\langle \pi_k, \pi_k \rangle_w}} = (x - \alpha_k)\, \tilde{\pi}_k - \beta_k \tilde{\pi}_{k-1} \sqrt{\frac{\langle \pi_{k-1}, \pi_{k-1} \rangle_w}{\langle \pi_k, \pi_k \rangle_w}}$$

$$\tilde{\pi}_{k+1}\sqrt{\beta_{k+1}} = (x - \alpha_k)\, \tilde{\pi}_k - \beta_k \tilde{\pi}_{k-1} \sqrt{\beta_k^{-1}} = (x - \alpha_k)\, \tilde{\pi}_k - \tilde{\pi}_{k-1}\sqrt{\beta_k}.$$

This gives us the three-term recurrence from Theorem 17 for all $k = 1, 2, \ldots$. □

2.3.1 Jacobi Matrix and it's eigenvalue decomposition

The coefficients of three-term recurrence can be arranged into a three diagonal symmetric matrix. This matrix has useful ties to the recurrence itself yielding valuable ties between its eigenvalue decomposition and to the roots of orthogonal polynomials.

Definition 18 ([5, Definition 1.30])**.** With reference to three-term recurrence in Theorem 17, the $n \times n$ Jacobi matrix associated with the first n orthonormal polynomials is symmetric, tridiagonal matrix

$$J_n := \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_n} \\ 0 & & & \sqrt{\beta_n} & \alpha_n \end{bmatrix}.$$

Theorem 19 (Roots of monic polynomials [5, Theorem 1.19])**.** *The monic polynomial $\pi_n \in P_n^m$ of degree n, generated by the three-term recurrence relation from Theorem 15, has exactly n unique real roots. We will denote these roots by $\boldsymbol{\tau}^{(n)} = \left[\tau_0^{(n)}, \dots, \tau_{n-1}^{(n)}\right]$.*

The eigenvalue decomposition of the symmetric Jacobi matrix J_n yields set of real eigenvalues. Specifically, if J_n denotes the n-th Jacobi matrix, its spectral decomposition is given by $J_n = Q_n \Lambda_n Q_n^T$, where Λ_n is a diagonal matrix containing the real eigenvalues of J_n, and Q_n is an orthonormal matrix ($Q_n^T Q_n = Q_n Q_n^T = I$) whose columns are the corresponding normalized eigenvectors.

For showing the ties between Jacobi matrix and orthonormal polynomials, we need to define a vector of orthonormal polynomials. For a sequence $\{\tilde{\pi}_i(x)\}_{i=0}^{n-1}$ consisting of the first n orthonormal polynomials generated with respect to the inner product $\langle \cdot, \cdot \rangle_w$ (each polynomial $\tilde{\pi}_i(x), i = 0, \dots, n-1$ has degree i) we define the corresponding vector of these orthonormal polynomials as:

$$\tilde{\boldsymbol{\pi}}(x) = \left[\tilde{\pi}_0(x), \tilde{\pi}_1(x), \dots, \tilde{\pi}_{n-1}(x)\right]^T.$$

This vector provides an orthonormal basis for the space of polynomials of degree at most $n-1$, denoted P_{n-1}.

Theorem 20 ([5, Theorem 1.31])**.** *The roots $\tau_j^{(n)}, j = 0, 1, \dots, n-1$, of π_n are the eigenvalues of the Jacobi matrix J_n. Furthermore, the vectors $\tilde{\boldsymbol{\pi}}\left(\tau_j^{(n)}\right)$ are corresponding eigenvectors, where $\tilde{\boldsymbol{\pi}}(x) = \left[\tilde{\pi}_0(x), \tilde{\pi}_1(x), \dots, \tilde{\pi}_{n-1}(x)\right]^T$, i.e., for each $j = 0, 1, \dots, n-1$:*

$$\tau_j^{(n)} \tilde{\boldsymbol{\pi}}(\tau_j^{(n)}) = J_n \tilde{\boldsymbol{\pi}}(\tau_j^{(n)}).$$

Proof. If the first n equations from Theorem 17 are written in the form

$$x\tilde{\pi}_k(x) = \sqrt{\beta_k}\tilde{\pi}_{k-1}(x) + \alpha_k\tilde{\pi}_k(x) + \sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(x),\ k = 0, 1, \dots, n-1,$$

$$\tilde{\pi}_{-1}(x) = 0,$$

and we recall

$$\tilde{\boldsymbol{\pi}}(x) = [\tilde{\pi}_0(x), \tilde{\pi}_1(x), \dots, \tilde{\pi}_{n-1}(x)]^T,$$

then we can express these equations for $k = 0, 1, \dots n-1$ in matrix form as

$$x\tilde{\boldsymbol{\pi}}(x) = J_n\tilde{\boldsymbol{\pi}}(x) + \sqrt{\beta_n}\tilde{\pi}_n(x)\boldsymbol{e}_n,$$

where $\boldsymbol{e}_n = [0, 0, \dots, 1]^T$ is the n-th coordinate vector in $\mathbb{R}^n$. The assertions from Theorem 20 regarding $\tau_j^{(n)}$ and $\tilde{\boldsymbol{\pi}}\left(\tau_j^{(n)}\right)$ follow immediately from this matrix equation by substituting $x = \tau_j^{(n)}$, where $\tau_j^{(n)}$ are roots of monic polynomial π_n and noting that $\tilde{\boldsymbol{\pi}}(\tau_j^{(n)}) \neq \mathbf{0}$ (since its first component $\tilde{\pi}_0(\tau_j^{(n)}) = 1/\sqrt{\beta_0} \neq 0$), yields:

$$\tau_j^{(n)}\tilde{\boldsymbol{\pi}}(\tau_j^i) = J_n\tilde{\boldsymbol{\pi}}(\tau_j^{(n)}) + \sqrt{\beta_n}\tilde{\pi}_n(\tau_j^{(n)})e_n.$$

Since $\tau_j^{(n)}$ are the roots of π_n, we have $\tilde{\pi}_n\left(\tau_j^{(n)}\right) = \pi_i\left(\tau_j^{(n)}\right) / \|\pi_i\|_w = 0$, and the equation simplifies to:

$$\tau_j^{(n)}\tilde{\boldsymbol{\pi}}(\tau_j^{(n)}) = J_n\tilde{\boldsymbol{\pi}}(\tau_j^{(n)}).$$

This shows that $\left(\tau_j^{(n)}, \tilde{\boldsymbol{\pi}}(\tau_j^{(n)})\right)$ are the eigenpairs of the Jacobi matrix J_n. □

Remark 21. Note that $\tilde{\boldsymbol{\pi}}(\tau_j^{(n)})$ are not necessarily normalized polynomials.

Corollary 22 (to Theorem 20 [5, Corollary to 1.31])**.** *Let $\boldsymbol{v}_j^{(n)}$ denote the normalized eigenvector of J_n corresponding to the eigenvalue $\tau_j^{(n)}$, and let $\boldsymbol{v}_{j,0}^{(n)}$ denote its first component. These satisfy:*

$$J_n\boldsymbol{v}_j^{(n)} = \tau_j^{(n)}\boldsymbol{v}_j^{(n)}, \quad \left(\boldsymbol{v}_j^{(n)}\right)^T\boldsymbol{v}_j^{(n)} = 1.$$

Then, for $j = 0, 1, \dots, n-1$:

$$\beta_0\left(\boldsymbol{v}_{j,0}^{(n)}\right)^2 = \frac{1}{\sum_{k=0}^{n-1}\left[\tilde{\pi}_k(\tau_j^{(n)})\right]^2}.$$

Proof. Recall the vector $\tilde{\boldsymbol{\pi}}(x) = [\tilde{\pi}_0(x), \tilde{\pi}_1(x), \dots, \tilde{\pi}_{n-1}(x)]$ from Theorem 20. For each normalized eigenvector $\boldsymbol{v}_j^{(n)}$:

$$\boldsymbol{v}_j^{(n)} = \left(\sum_{k=0}^{n-1}\left[\tilde{\pi}_k(\tau_j^{(n)})\right]^2\right)^{-1/2}\tilde{\boldsymbol{\pi}}(\tau_j^{(n)}), \quad j = 0, 1, \dots, n.$$

Noting from Theorem 17 that $\tilde{\pi}_0 = 1/\sqrt{\beta_0}$ is constant, if we compare the first component of each side of the vector equation above and square the resulting scalar equation, we obtain:

$$\left(\boldsymbol{v}_{j,0}^{(n)}\right)^2 = \left(\sum_{k=0}^{n-1} \left[\tilde{\pi}_k(\tau_j^{(n)})\right]^2\right)^{-1} \frac{1}{\beta_0}, \quad j = 0, 1, \ldots, n.$$

Rearranging this gives the desired relationship:

$$\beta_0 \left(\boldsymbol{v}_{j,0}^{(n)}\right)^2 = \frac{1}{\sum_{k=0}^{n-1} \left[\tilde{\pi}_k(\tau_j^{(n)})\right]^2}, \quad j = 0, 1, \ldots, n.$$

□

2.4 Quadrature rules

Numerical quadrature provides an effective methodology for approximating the value of definite and improper integrals. The integral approximation is calculated as the weighted sum of the integrated function evaluated at the nodes. Specifically, Gaussian quadrature rules, which are inherently linked to orthogonal polynomials, offer high accuracy. This section introduces the process of deriving the quadrature nodes $\{\tau_i\}_{i=1}^N$ and corresponding weights $\{\lambda_i\}_{i=1}^N$.

For more details on numerical approximation of integrals, we refer to [8] and [9].

Definition 23 (The Quadrature rule)**.** A quadrature rule is a set of weights λ_j and nodes τ_j, $j = 1, 2, \ldots, n$, used to approximate the value of a weighted integral:

$$\int_I f(x)w(x)\,dx \approx \sum_{j=1}^n \lambda_j f(\tau_j).$$

Theorem 24 ([5, Theorem 1.45])**.** *Consider a quadrature rule for approximating weighted integral $\int_I f(x)w(x)\,dx$ using n distinct nodes $\tau_1, \ldots, \tau_n$, where $w(x)$ is a positive weight function defining an inner product $\langle \cdot, \cdot \rangle_w$. Let this quadrature rule satisfy two conditions:*

1. The rule is interpolatory, meaning it is derived by integrating the Lagrange interpolating polynomial based on the nodes τ_j. The approximation is given by:

$$\int_I f(x)w(x)\,dx \approx \sum_{j=1}^n \lambda_j f(\tau_j),$$

where the weights λ_j are the integrals of the Lagrange basis polynomials:

$$\lambda_j = \int_I l_j(x)w(x)\,dx, \tag{2.3}$$

where $l_j(x)$ are the Lagrange basis polynomials:

$$l_j(x) = \prod_{\substack{\mu=1 \\ \mu \neq j}}^{n} \frac{x - \tau_\mu}{\tau_j - \tau_\mu}.$$

2. The node polynomial $\omega_n(x) = \prod_{j=1}^{n}(x - \tau_j)$, is orthogonal to all polynomials $p(x)$ of degree less than n with respect to the weight function $w(x)$. That is:

$$\int_I w(x)\omega_n(x)p(x)\,dx = 0,$$

for all $p \in P_{n-1}$.

If both conditions hold, then the nodes $\tau_1, \ldots, \tau_n$ of the quadrature rule are precisely the roots of the n-th degree orthogonal polynomial $\pi_n(x)$ associated with the weight function $w(x)$ and correspondingly the inner product $\langle \cdot, \cdot \rangle_w$.

Remark 25 ($2n-1$ quadrature exactness [5, pg. 8])*.* The n-point Gauss quadrature rule integrates polynomials of degree up to $2n-1$ exactly.

2.5 Golub-Welsch algorithm

Having established that the roots of the orthogonal polynomial π_n correspond to the eigenvalues of the associated Jacobi matrix J_n, the focus now shifts to the computation of the corresponding quadrature weights. This section details the procedure for determining these weights, employing the well-established Golub-Welsch algorithm [4], which utilizes the first components of the normalized eigenvectors.

Theorem 26 (Gauss Quadrature from eigenvectors [5, Theorem 3.1])**.** *The nodes τ_j, $j = 1, 2, \ldots, n$, of the n-point Gauss quadrature rule associated with the inner product $\langle \cdot, \cdot \rangle_w$ are the eigenvalues of the Jacobi matrix J_n. The corresponding weights $\lambda_j, j = 1, 2, 3, \ldots, n$, are given by:*

$$\lambda_j = \beta_0 \boldsymbol{v}_{j,1}^2,$$

where $\beta_0 = \int_I w(x)\,dx$ and $\boldsymbol{v}_{j,1}$ is the first component of the normalized eigenvector $\boldsymbol{v}_j$ of J_n corresponding to the eigenvalue τ_j.

Proof. [5, page 153] Let us recall a vector of orthonormal polynomials

$$\tilde{\boldsymbol{\pi}}(x) = \left[\tilde{\pi}_0(x), \tilde{\pi}_1(x), \ldots, \tilde{\pi}_{n-1}(x)\right]^T.$$

From Corollary 22 we have:

$$\beta_0 \boldsymbol{v}_{j,1}^2 = \frac{1}{\sum_{k=0}^{n-1} \left[\tilde{\pi}_k(\tau_j^{(n)})\right]^2}, \quad j = 1, \dots, n,$$

where $\boldsymbol{v}_{j,1}$ is the first component of the normalized eigenvector $\boldsymbol{v}_j$ corresponding to the eigenvalue $\tau_j^{(n)}$. Next, let $f(x) = \tilde{\pi}_k(x)$ for some $k \in \{0, 1, \dots, n-1\}$. The n-point Gauss quadrature rule integrates polynomials of degree up to $2n-1$ exactly, see Remark 25. Since $f(x)$ is a polynomial of degree $k \leq n-1 < 2n-1$, the Gauss formula is exact:

$$\int\limits_I \tilde{\pi}_k(x) w(x)\, dx = \sum_{j=1}^{n} \lambda_j^G \tilde{\pi}_k(\tau_j^G), \quad k = 0, 1, \dots, n-1.$$

The integral on the left side is $\int_I \tilde{\pi}_k(x) w(x)\, dx = \langle \tilde{\pi}_k, 1 \rangle_w$. Since $1 = \sqrt{\beta_0}\tilde{\pi}_0(x)$ (because $\tilde{\pi}_0$ is the constant orthonormal polynomial, $\tilde{\pi}_0 = 1/||\pi_0||_w = 1/\sqrt{\langle 1, 1\rangle_w} = 1/\sqrt{\beta_0}$), this integral becomes $\sqrt{\beta_0}\langle \tilde{\pi}_k, \tilde{\pi}_0 \rangle_w = \sqrt{\beta_0}\delta_{k,0}$ by the orthonormality of the $\tilde{\pi}$ polynomials. Thus, the exact Gauss formula yields:

$$\beta_0^{1/2} \delta_{k,0} = \sum_{j=1}^{n} \lambda_j^G \tilde{\pi}_k(\tau_j^G), \quad k = 0, 1, \dots, n-1,$$

where $\delta_{k,0}$ is the Kronecker delta. This system of equations can be written in matrix form as:

$$P^T \boldsymbol{\lambda}^G = \beta_0^{1/2} \boldsymbol{e}_1, \tag{2.4}$$

where P is the $n \times n$ matrix whose $(k+1, j)$ entry is $\tilde{\pi}_k(\tau_j^G)$, $\boldsymbol{\lambda}^G$ is the vector of Gauss weights $[\lambda_1^G, \dots, \lambda_n^G]^T$ and $\boldsymbol{e}_1 = [1, 0, \dots, 0]^T \in \mathbb{R}^n$ is the first standard basis vector. From Theorem 20 we know that the columns of P are eigenvectors, therefore mutually orthogonal, and specifically:

$$PP^T = D_\pi = \begin{bmatrix} d_0 & & & \\ & d_1 & & \\ & & \ddots & \\ & & & d_{n-1} \end{bmatrix}, \quad d_{j-1} = \sum_{k=0}^{n-1} \left[\tilde{\pi}_k(\tau_j^{(n)})\right]^2$$

Multiplying the equation (2.4) by P from the left yields:

$$D_\pi \boldsymbol{\lambda}^G = \beta_0^{1/2} P \boldsymbol{e}_1.$$

Since the first row of P consists of $\tilde{\pi}_0(\tau_j^G)$ and from Theorem 17 we have $\tilde{\pi}_0(x) = \beta_0^{-1/2}$, then

$$\beta_0^{1/2} P \boldsymbol{e}_1 = \beta_0^{1/2} \beta_0^{-1/2} \boldsymbol{e} = \boldsymbol{e},$$

where $\boldsymbol{e} = [1, 1, \ldots, 1]^T \in \mathbb{R}^n$. There follows $\lambda^G = D_\pi^{-1}\boldsymbol{e}$, that is, for each $j = 1, \ldots, n$:

$$\lambda_j^G = \frac{1}{d_{j-1}} = \frac{1}{\sum_{k=0}^{n-1} \left[\tilde{\pi}_k(\tau_j^{(n)})\right]^2},$$

by Corollary 22 yielding $\lambda_j^G = \beta_0 \boldsymbol{v}_{j,1}^2$. □

2.6 Generalization of Legendre polynomials and quadrature

This work focuses specifically on Legendre polynomials because they can be adapted for integration over any finite interval $\langle a, b\rangle$. Such integration can be achieved by applying an affine transformation to the Legendre polynomials and their corresponding quadrature nodes and weights.

For more information on affine transformations, we refer to [10].

Remark 27. Let the orthogonal polynomials denoted by $\pi_i^L(x)$ (the Legendre polynomials) be defined with respect to the inner product over the interval $I^L = \langle -1, 1\rangle$ with the weight function $w(x) = 1$. Consider an interval $I = \langle a, b\rangle$, where $a, b \in \mathbb{R}$ and $a < b$. For the inner product defined over the interval I with the weight function $w(x) = 1$, the corresponding orthogonal polynomials $\pi_i(x)$ are related to $\pi_i^L(x)$ by $\pi_i(x) = \pi_i^L\left(\frac{a+b}{a-b} + \frac{2}{b-a}x\right)\sqrt{\frac{2}{b-a}}$. Additionally, this transformation preserves the normalization of the basis, i.e. if $\tilde{\pi}_i^L$ are the orthonormal Legendre polynomials, then the polynomials defined by $\tilde{\pi}_i(x) = \tilde{\pi}_i^L\left(\frac{a+b}{a-b} + \frac{2}{b-a}x\right)\sqrt{\frac{2}{b-a}}$ are also orthonormal.

Proof. We will prove the orthogonality of the polynomials $\pi_i(x)$ and $\pi_j(x)$ for $i \neq j$ with respect to the inner product $\langle \cdot, \cdot \rangle_1 = \int_a^b u(x)v(x)dx$. Recall the relationship $\pi_k(x) = \pi_k^L\left(\frac{a+b}{a-b} + \frac{2}{b-a}x\right)\sqrt{\frac{2}{b-a}}$, where π_k^L are Legendre polynomials. Thus, for $i \neq j$:

$$\langle \pi_i, \pi_j \rangle_1 = \int\limits_a^b \pi_i(x)\pi_j(x)\,dx = \int\limits_a^b \pi_i^L\left(\frac{a+b}{a-b} + \frac{2}{b-a}x\right)\pi_j^L\left(\frac{a+b}{a-b} + \frac{2}{b-a}x\right)\frac{2}{b-a}\,dx.$$

Let us perform the substitution:

$$\hat{x} = \frac{a+b}{a-b} + \frac{2}{b-a}x.$$

Then $d\hat{x} = \frac{2}{b-a}dx$. The limits change as follows: when $x = a$, $\hat{x} = -1$, and when $x = b$, $\hat{x} = 1$. Substituting into the integral gives:

$$\int\limits_a^b \pi_i^L(\ldots)\,\pi_j^L(\ldots)\,\frac{2}{b-a}dx = \int\limits_{-1}^1 \pi_i^L(\hat{x})\,\pi_j^L(\hat{x})\,d\hat{x}.$$

Since π_i^L and π_j^L are orthogonal Legendre polynomials for $i \neq j$ with respect to the weight $w(x) = 1$ on $[-1, 1]$, the integral is zero:

$$\int_{-1}^{1} \pi_i^L(\hat{x})\, \pi_j^L(\hat{x})\, d\hat{x} = 0.$$

Therefore, $\langle \pi_i, \pi_j \rangle_1 = 0$ for $i \neq j$. If the polynomials π_i^L are orthonormal then π_i are also orthonormal. □

Theorem 28 ([5, Theorem 1.47])**.** *The weights λ_j for an n-point quadrature rule approximating $\int_a^b f(x)\, w(x)\, dx$, using the roots τ_i $(i = 0, \ldots, n-1)$ of the corresponding orthogonal polynomial as nodes (eq.* (2.3)*), are given by:*

$$\lambda_j = \frac{\int_a^b \prod_{i\neq j, i=0}^{n-1} (x - \tau_i)\, dx}{\prod_{i\neq j, i=0}^{n-1} (\tau_j - \tau_i)}, \quad j = 0, \ldots, n-1.$$

Remark 29. Let τ_i^L denote the roots of Lagrange polynomials and λ_i^L denote the corresponding Gauss-Legendre quadrature weights. For orthogonal polynomials $\pi(x)$ associated with the inner product over the interval $I = \langle a, b \rangle$ (with weight $w(x) = 1$), the roots (Gauss quadrature nodes) are $\tau_i = \frac{a+b}{2} + \frac{b-a}{2}\tau_i^L$ and the weights are $\lambda_i = \frac{b-a}{2}\lambda_i^L$.

Proof. Let τ_i^L be the roots of the n-th degree Legendre polynomial π_n^L, then $\pi^L(\tau_i^L) = 0$ for all $i = 0, \ldots, n-1$. From Remark 27 we have the polynomial $\pi_n(x) = \pi_n^L\left(\frac{a+b}{a-b} + \frac{2}{b-a}x\right)\sqrt{\frac{2}{b-a}}$. The roots τ_i of the polynomial π_n must satisfy $\pi_n(\tau_i) = 0$. This implies:

$$\pi_n^L\left(\frac{a+b}{a-b} + \frac{2}{b-a}\tau_i\right) = 0.$$

Since τ_i^L are the roots of π_n^L, we must have:

$$\tau_i^L = \frac{a+b}{a-b} + \frac{2}{b-a}\tau_i \implies \frac{a+b}{2} + \frac{b-a}{2}\tau_i^L = \tau_i.$$

If we then utilize this substitution in Theorem 28 we get:

$$\begin{aligned}
\lambda_j &= \frac{\int_a^b \prod_{i\neq j,i=0}^{n-1} (x-\tau_i)\ dx}{\prod_{i\neq j,i=0}^{n-1} (\tau_j-\tau_i)} = \\
&= \frac{\int_a^b \prod_{i\neq j,i=0}^{n-1} \left(x-\frac{a+b}{2}-\frac{b-a}{2}\tau_i^L\right)\ dx}{\prod_{i\neq j,i=0}^{n-1} \left(\frac{a+b}{2}+\frac{b-a}{2}\tau_j^L-\frac{a+b}{2}-\frac{b-a}{2}\tau_i^L\right)} = \\
&= \frac{\int_{-1}^1 \frac{b-a}{2} \prod_{i\neq j,i=0}^{n-1} \left(\frac{a+b}{2}+\frac{b-a}{2}\hat{x}-\frac{a+b}{2}-\frac{b-a}{2}\tau_i^L\right)\ d\hat{x}}{\prod_{i\neq j,i=0}^{n-1} \left(\frac{b-a}{2}\left(\tau_j^L-\tau_i^L\right)\right)} = \\
&= \frac{\left(\frac{b-a}{2}\right)^n \int_{-1}^1 \prod_{i\neq j,i=0}^{n-1} \left(\hat{x}-\tau_i^L\right)\ d\hat{x}}{\left(\frac{b-a}{2}\right)^{n-1} \prod_{i\neq j,i=0}^{n-1} \left(\tau_j^L-\tau_i^L\right)} = \\
&= \frac{b-a}{2}\frac{\int_{-1}^1 \prod_{i\neq j,i=0}^{n-1} \left(\hat{x}-\tau_i^L\right)\ d\hat{x}}{\prod_{i\neq j,i=0}^{n-1} \left(\tau_j^L-\tau_i^L\right)} = \\
&= \frac{b-a}{2}\lambda_j^L.
\end{aligned}$$

□

2.7 Numerical experiments

In this section, we present numerical experiments demonstrating:

- assembly of orthogonal and orthonormal polynomials,
- the efficiency of construction of quadrature rule using Golub-Welsch algorithm,
- convergence of quadrature approximation for various types of functions.

all numerical results presented were generated using the implementation provided in [1].

2.7.1 Polynomials

Legendre polynomials are generated using the three-term recurrence relation presented in Theorem 15. This can be done efficiently using Numpy array operations. The first six polynomials in this sequence are illustrated in Figure 2.1.

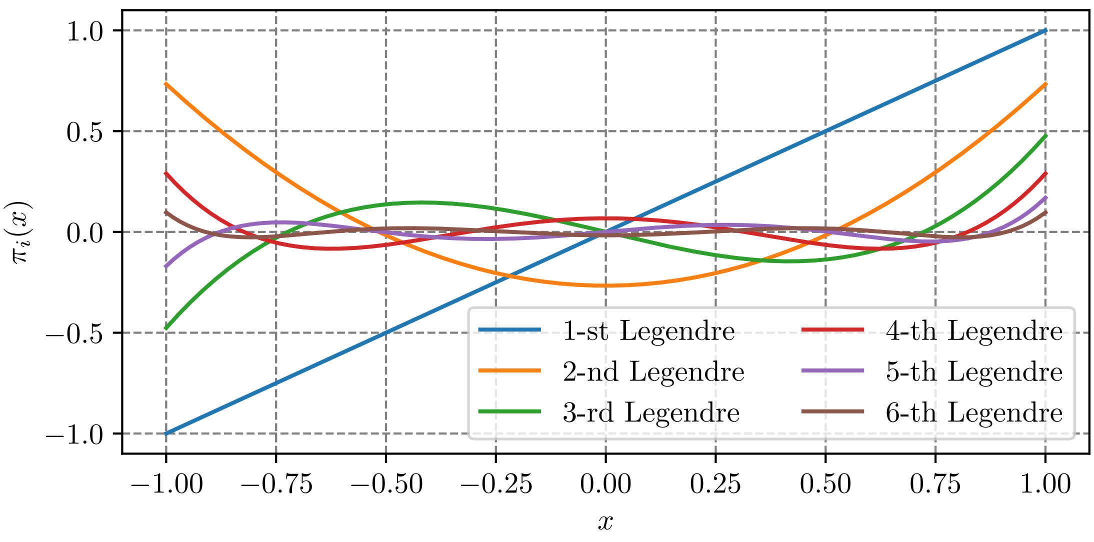

Figure 2.1: Monic Legendre polynomials

Normalized Legendre polynomials are generated using the recurrence relation described in Theorem 17. Similarly, the first six polynomials in this normalized sequence are shown in Figure 2.2.

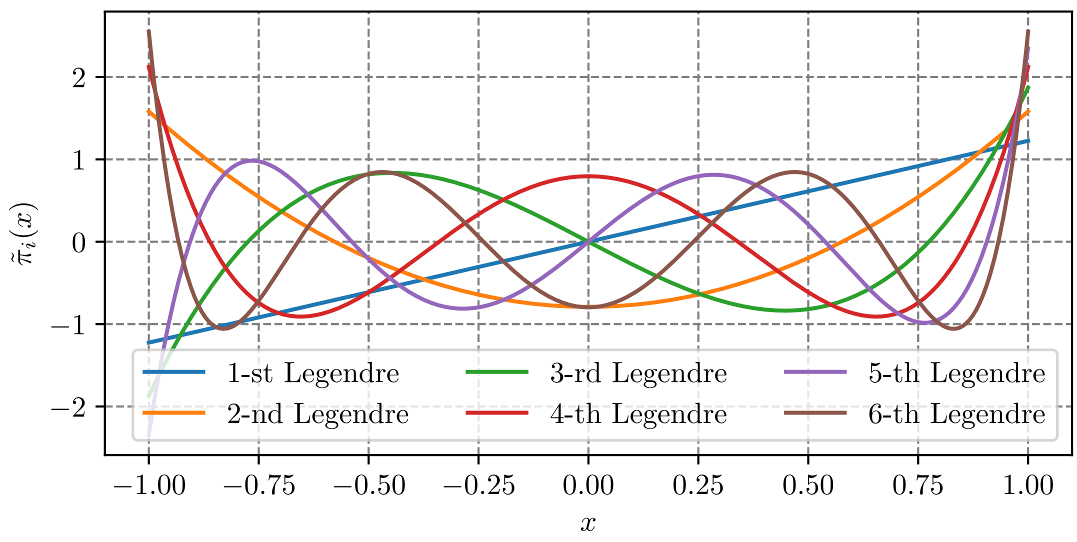

Figure 2.2: Normalized Legendre polynomials

The normalized Legendre polynomials were also adapted for use on a different interval, applying the affine transformation described in Remark 27.

2.7.2 Quadrature rules

The focus now shifts to Gaussian quadrature rules and their use for approximations of definite integrals over finite intervals.

First, the computational time required to obtain the quadrature nodes and weights is examined. This computation involves determining the eigenpairs of the Jacobi matrix J_n and its construction and is performed using the Golub-Welsch algorithm. The Jacobi matrix J_n is represented in the code as two one-dimensional arrays: the main diagonal and the first sub-diagonal. These arrays are then used in a function ‘eigh_tridiagonal‘ from the ‘scipy.linalg‘ library to calculate the eigenvalues and eigenvectors. From Theorem 26, we know that the eigenvalues are the quadrature nodes and the weights can be obtained from the first components of the eigenvectors. Figure 2.3 illustrates the relationship between the size n of the Jacobi matrix J_n (where n is also the number of nodes and weights obtained) and the time taken to compute these nodes and weights. It is a log-log graph where we observe that the data points can be approximated by a linear fit with a slope close to 2, suggesting that the computation time has approximately quadratic complexity.

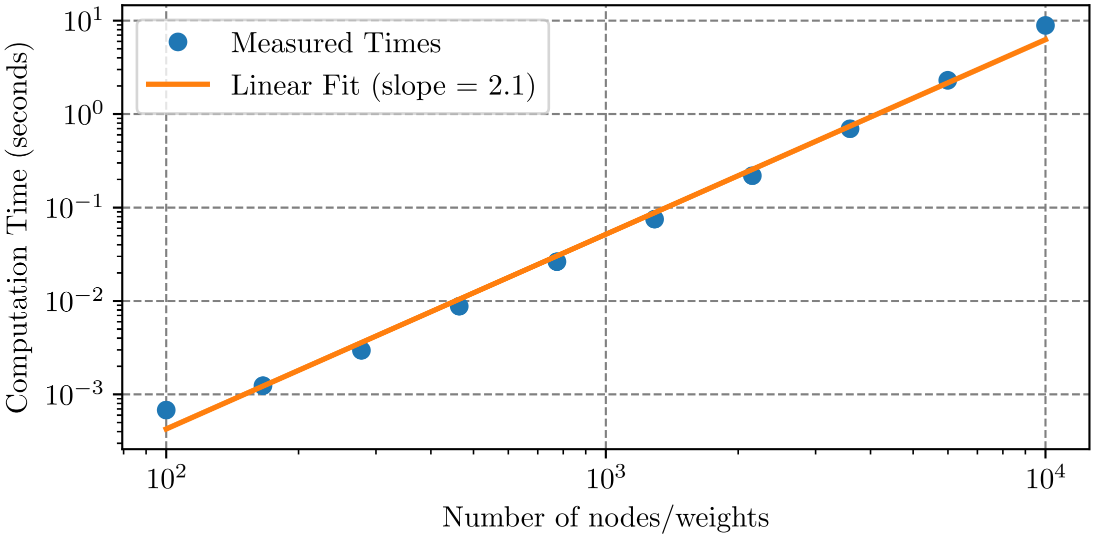

Figure 2.3: Log-Log Plot of Computation Time vs. Jacobi Size n

We will now try to experiment with different functions and examine the approximation error $|i_n - i^*|$, where i_n is the integral approximation obtained using n nodes and weights, and i^* is the exact value of the integral.

Example 30. We will approximate the integral of a polynomial. Specifically, we will consider the polynomial $f(x) = x^{50} + x^4 - 4x^3 - 15x + 35$. The exact value of the integral in this case will is $i^* = \frac{17962}{255}$. Figure 2.4 shows the polynomial $f(x)$ on the left side and the convergence graph of the approximation error on the right side. We observe the expected convergence to machine precision at $n = 26$ nodes/weights, because we know from Remark 25 that a Gaussian quadrature rule with n nodes integrates polynomials of degree up to $2n - 1$ exactly.

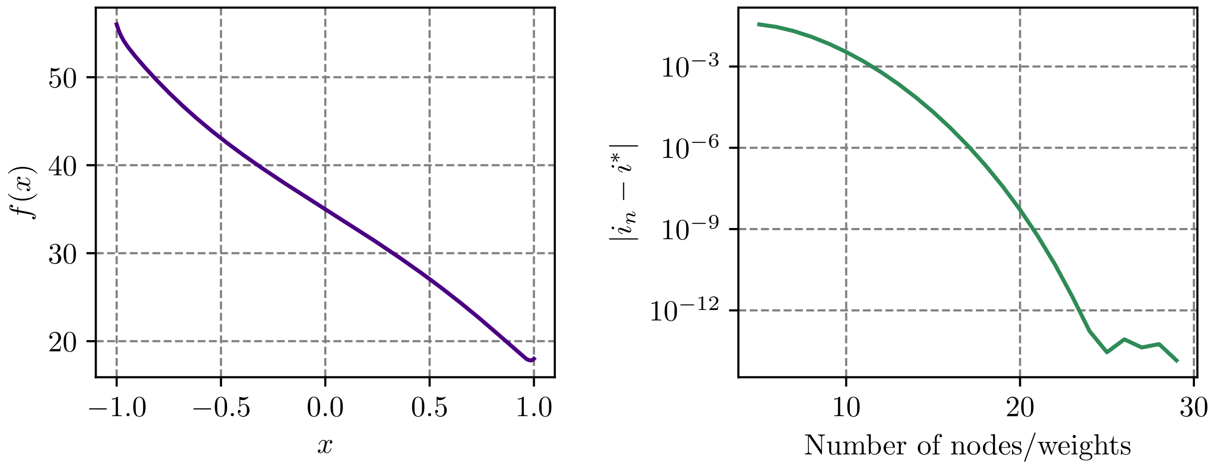

Figure 2.4: Integrated function (left) and the convergence of numerical integration (right)

Example 31. Next, we will approximate the integral of the smooth function $f(x) = \cos(x^2)$. Figure 2.5 shows $f(x)$ on the left and convergence graph of the approximation error on the right side. The exact solution is tied to Fresnel integral (C), and in practice is also computed numerically [11]. The exact value of the integral is $i^* = \sqrt{2\pi}C(\sqrt{\frac{2}{\pi}})$. Exponential convergence is observed in the right graph.

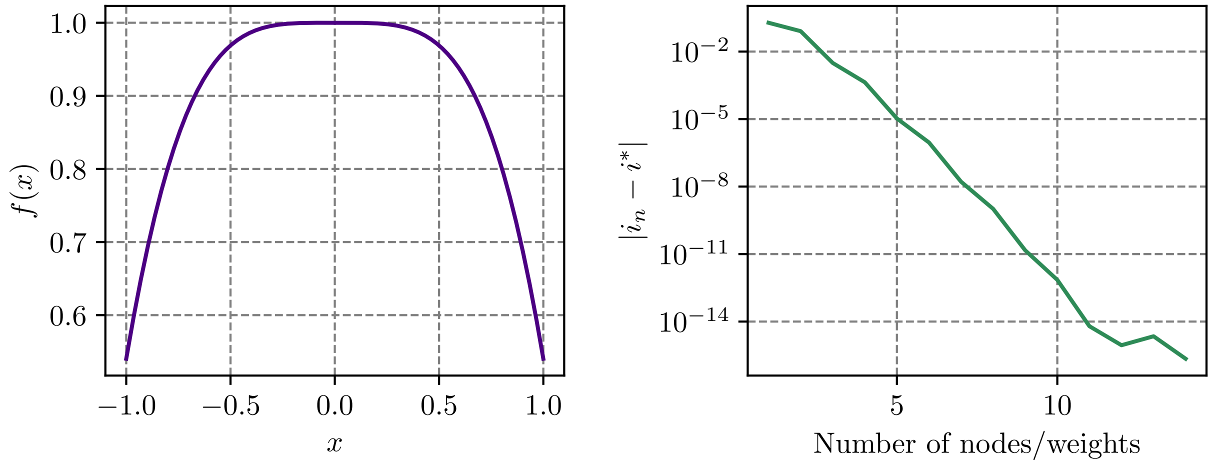

Figure 2.5: Integrated function (left) and the convergence of numerical integration (right)

Example 32. Here we experiment with an integral of a non-smooth function $f(x) = |x| + |x + 0.5| - |x - 0.5|$. The exact value of the integral is $i^* = 1$. Figure 2.6 shows this function and the corresponding quadrature approximation error for an increasing number of nodes. A noticeable pattern in the error can be observed: its value fluctuates depending on whether an odd or even number of nodes and weights is used. The overall accuracy of the approximation is also lower than typically achieved for smooth functions. This behavior is expected because the effectiveness of Gaussian quadrature depends on the smoothness of the function being integrated, and $f(x)$ has points where it is not differentiable within the interval I. In order to achieve a better approximation, we could split the interval I into multiple subintervals such that the function is smooth on each subinterval, and then integrate the function separately over each respective subinterval. Note that in this case a quadrature consisting of two points would be enough for each of the four subintervals.

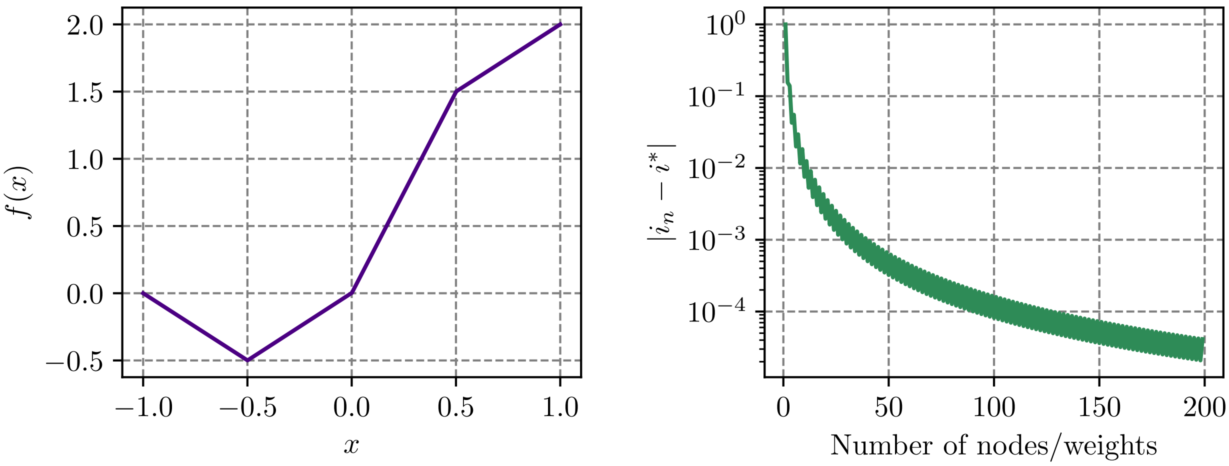

Figure 2.6: Integrated function (left) and the convergence of numerical integration (right)

Example 33. Figure 2.7 shows a discontinuous shifted sign function defined as:

$$f(x) = \begin{cases} -1 & \text{if } x < -0.5 \\ 0 & \text{if } x = -0.5 \\ 1 & \text{if } x > -0.5 \end{cases} .$$

The exact value of the integral is $i^* = 1$. We can observe that the accuracy of the quadrature approximation is even lower than for the previous non-smooth function, and the error fluctuates significantly depending on whether an odd or even number of nodes and weights is used. This occurs because $f(x)$ is discontinuous within the interval I (specifically at $x = -0.5$). We could again split the interval I into subintervals (e.g., at the point of discontinuity) to achieve a more accurate result. In this case, a one-point quadrature rule applied to each of the two subintervals would be sufficient to obtain the exact value of the integral.

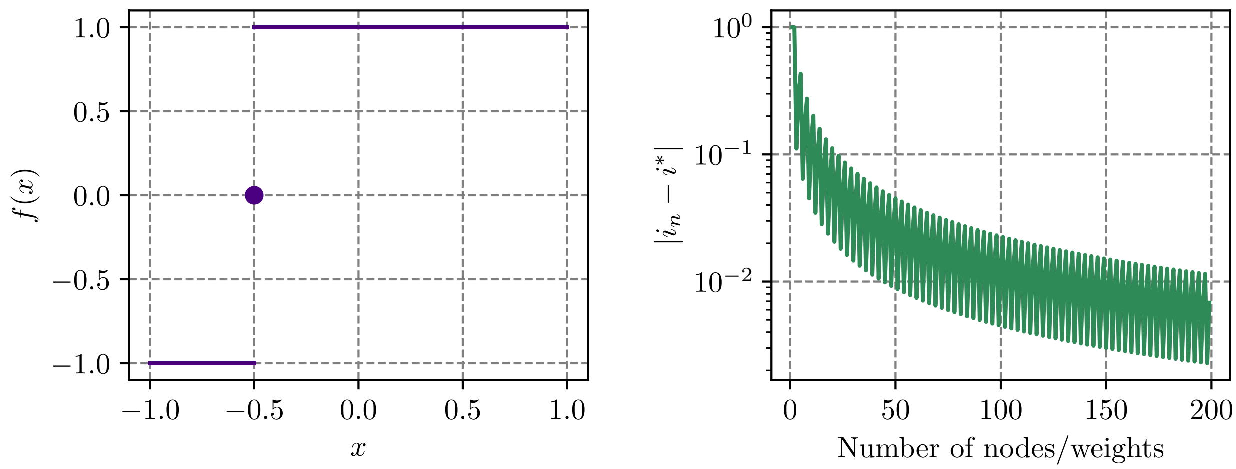

Figure 2.7: Integrated function (left) and the convergence of numerical integration (right)

Example 34. We will now experiment with two-dimensional integration. In this example, we will integrate the function $f(x, y) = \sin(x^2 + y^2)$ over domain $\mathcal{T} = \langle -1, 1\rangle \times \langle -1, 1\rangle$. The analytical evaluation of this definite integral involves the Fresnel integrals (C, S). In practice, this value is often computed numerically [11]. The exact value for this specific integral is $i^* = 4\pi C\left(\sqrt{\frac{2}{\pi}}\right) S\left(\sqrt{\frac{2}{\pi}}\right)$. Figure 2.8 shows the convergence of the quadrature error for this function for different numbers of weights and nodes used in each dimension. We observe that convergence to machine precision is achieved around $n = 11$ nodes per dimension.

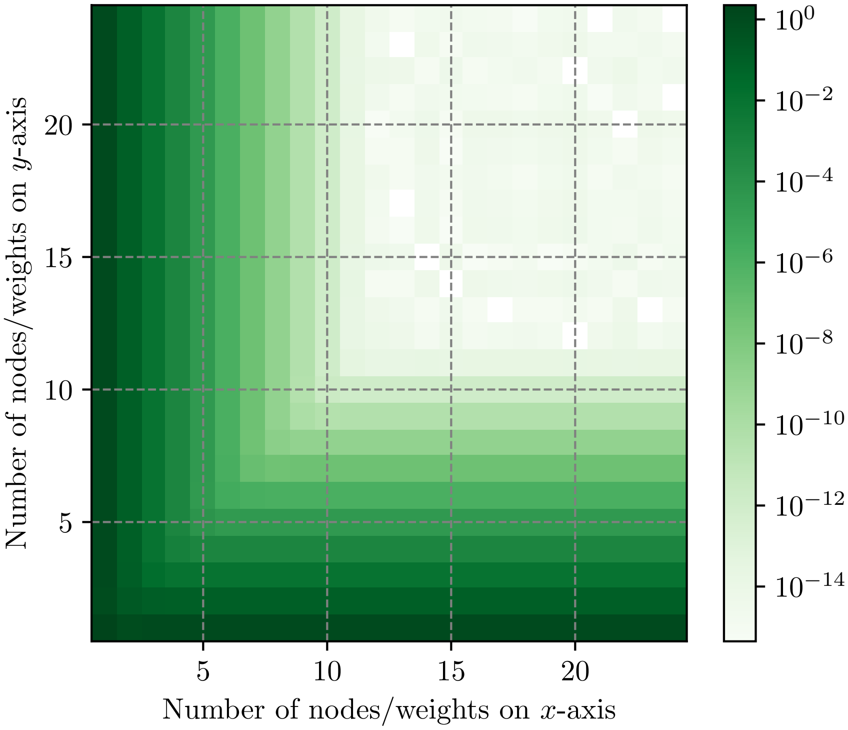

Figure 2.8: Convergence of 2D numerical integration

Example 35. In this example, we want to show how the convergence of the quadrature error appears for a non-symmetric function. We will integrate $f(x, y) = x^2 y^2 \cos(\pi(10x + y))$. Exact value of this integral is $i^* = -\frac{4}{25\pi^4}$. Figure 2.9 shows the convergence of the quadrature error for different numbers of weights and nodes used in each dimension. We observe that convergence to machine precision is achieved around $n_x = 34$ nodes for the x-dimension and $n_y = 11$ nodes for the y-dimension

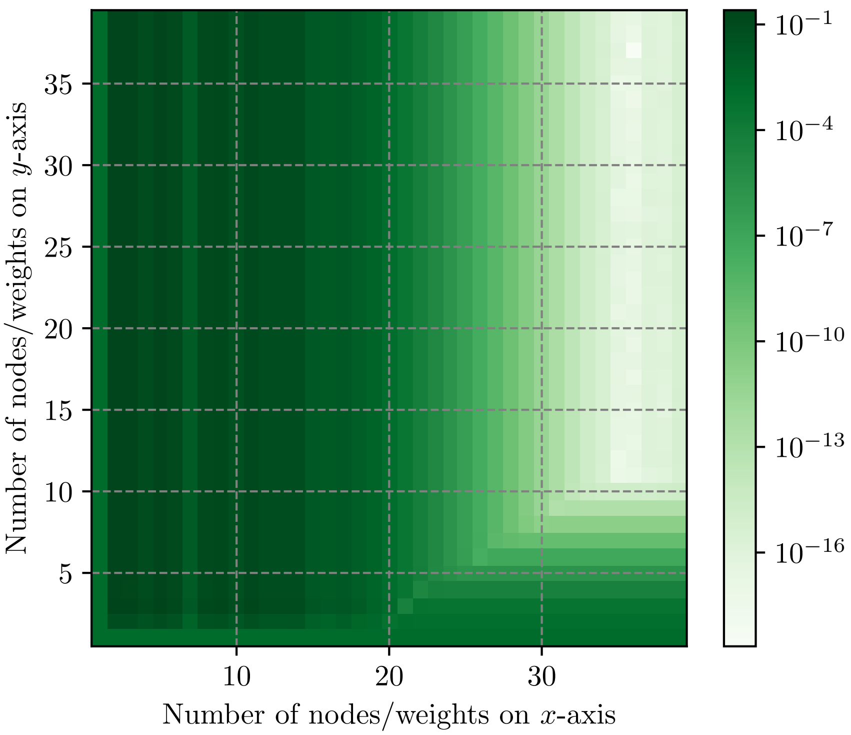

Figure 2.9: Convergence of 2D numerical integration

Chapter 3

Probability

This chapter starts with an introduction to the Hilbert space $L^2(I)$. To keep the thesis approachable, we constructed $L^2(I)$ as a completion of the space of continuous functions $C(I)$ with respect to the L^2 norm defined on the interval I. After this, key ideas from probability theory are introduced. This includes foundational elements of measure theory, the axiomatic definition of a probability space, and the concept of expected value. Building upon this foundation, the discussion then progresses to the topic of stochastic processes, introducing the concepts of random fields, their associated autocovariance functions, and the important subclass represented by Gaussian random fields (GRF).

For more details considering the basics of functional analysis and measure theory, please refer to [12, 13]. More details on probability theory can be found in [14, 15].

3.1 L^2 space

Definition 36 (L^2 norm)**.** For an interval $I = \langle a, b\rangle$, where $a, b \in \mathbb{R}, a < b$, the L^2-norm on $C(I)$ is defined as

$$\|f\|_{L^2} \coloneqq \left(\int\limits_I |f(x)|^2 \, dx \right)^{1/2} .$$

Definition 37 (Cauchy sequence)**.** Let $\{f_i\}_{i=0}^{\infty}$ be a sequence of functions in $C(I)$, where $I = \langle a, b\rangle$. This sequence is called a Cauchy sequence with respect to the L^2-norm $\|\cdot\|_{L^2}$, if for every $\varepsilon > 0$ there exists an integer N such that for all integers $m, n \geq N$, we have

$$\|f_n - f_m\|_{L^2} < \varepsilon.$$

Definition 38 ($\mathcal{L}^2$ set)**.** Let $\mathcal{L}^2(I)$ denote the set of all Cauchy sequences $\{f_i\} \subset C(I)$ with respect to the L^2-norm.

Definition 39 (Equivalence class)**.** We call two Cauchy sequences $\{f_i\}, \{g_i\} \in \mathcal{L}^2(I)$ equivalent if

$$\lim_{i\to\infty} \|f_i - g_i\|_{L^2} = 0.$$

The set of all sequences equivalent to a given sequence $\{f_i\}$ is called an equivalence class and is denoted by $[\{f_i\}]$.

Definition 40 (L^2 Space)**.** Let $F := \{f_i\}_{i=0}^{\infty} \in \mathcal{L}^2(I)$ and $G := \{g_i\}_{i=0}^{\infty} \in \mathcal{L}^2(I)$. Let us define the space $L^2(I)$ as an equivalence class space on $\mathcal{L}^2(I)$, representing the completion of $C(I)$ with respect to the L^2-norm:

$$L^2(I) := \left\{[F] : F \in \mathcal{L}^2(I)\right\}.$$

add a norm

$$\|[F]\|_{L^2} := \lim_{i\to\infty} \|f_i\|_{L^2}$$

and an inner product

$$\langle [F], [G] \rangle_{L^2} := \lim_{i\to\infty} \int\limits_I f_i(x)\, g_i(x)\, dx.$$

Corollary 41. *$L^2(I)$ is a Hilbert space. Also, this definition of $L^2(I)$ space yields the same space (isometrically isomorphic) as $L^2(I)$ under Lebesgue measure [13, section 7.4 Theorem 12].*

3.2 Probability fundamentals

Consider a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Ω is the sample space, i.e. it is the set of all possible outcomes. In general, the sample space is an abstract set, one large enough to parameterize all possible outcomes of the experiment. $\mathcal{F}$ is a collection of subsets of Ω and comprises of those subsets to which we can assign probabilities. Formally, it is a *σ-algebra*. Any measurable set, $F \in \mathcal{F}$ is known as an *event*. Each event corresponds to a set of outcomes in the experiment. The probability measure $\mathbb{P}$ assigns a probability, a number between 0 and 1, to every measurable set in $\mathcal{F}$.

Example 42. We can consider rolls of dice as an example of probability space $(\Omega, \mathcal{F}, \mathbb{P})$. In a roll of a die there are six possible outcomes and $\Omega = \{1, 2, 3, 4, 5, 6\}$. For a sequence of M rolls, the sample space is $\Omega = \{1, 2, 3, 4, 5, 6\}^M$. $\mathcal{F}$ is a collection of subsets of Ω, these subsets are known as events. Each event corresponds to a set of outcomes in the experiment. Let's say we want to know the probability of rolling an even number and so the set $F = \{2, 4, 6\}$ is included as an event in the σ-algebra $\mathcal{F}$. Lastly we have the probability measure $\mathbb{P}$, which assigns a probability to every measurable set in $\mathcal{F}$. Probability will be a number between zero and one, where zero means the event will never occur and one means the event will always occur. Higher probability means the event is more likely to occur in an experiment. For a fair dice roll the probability of rolling an even number would be $\mathbb{P}(\{2, 4, 6\}) = 1/2$.

Definition 43 (σ-algebra)**.** For a set Ω, we call a set $\mathcal{F}$, whose elements are subsets of Ω, a sigma σ-algebra if and only if it satisfies the following axioms:

1. $\Omega \in \mathcal{F}$,
2. If $A \in \mathcal{F}$, then $A^c \in \mathcal{F}$(where A^c is the complement of A, also denoted by $\Omega \setminus A$),
3. If $\{A_n\}$ is a countable collection of elements of $\mathcal{F}$ and $A = \bigcup_{n=1}^{\infty} A_n$, then $A \in \mathcal{F}$.

Definition 44 (Measure)**.** Let Ω be a set, and let $\varSigma$ be a σ-algebra on Ω (i.e., a collection of subsets of Ω containing Ω itself, closed under complements and countable unions). A function $\mu : \varSigma \to \langle 0, \infty \rangle$ is called a measure on the measurable space $(\Omega, \varSigma)$ if $\mu(\emptyset) = 0$ and for any countable collection $\{A_i\}$ of pairwise disjoint sets in $\varSigma$:

$$\mu\left(\bigcup_i A_i\right) = \sum_i \mu(A_i)\,.$$

.

Definition 45 (Probability measure [14, Definition 4.1])**.** A measure $\mathbb{P}$ on $(\Omega, \mathcal{F})$ is a *probability measure* if it has unit total mass, i.e., $\mathbb{P}(\Omega) = 1$.

Definition 46 (Probability space)**.** A probability space is a triple $(\Omega, \mathcal{F}, \mathbb{P})$, where Ω is a sample space, $\mathcal{F}$ is a sigma-algebra of events and $\mathbb{P}$ is a probability measure on $\mathcal{F}$.

3.3 Stochastic processes and random fields

This section defines stochastic processes and random fields, we will work only with real-valued variables. Further on, we discuss the covariance and the autocovariance function. The section concludes by explaining the meaning of stationarity for a stochastic process.

Definition 47 (Random variables, Realization [14, Definition 4.3])**.** For a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, a measurable map $X : \mathcal{F} \to \mathbb{R}$ is called a real-valued *random variable.*

Remark 48. The value $X(\omega)$ for a given outcome $\omega \in \Omega$ belongs to $\mathbb{R}$ and is called a *realization* of X.

Definition 49 (Random vector)**.** A random vector $\mathbb{X} \coloneqq (X_1, X_2, \ldots, X_n)$ is a vector whose elements $X_i, i = 1, 2, \ldots, n$ are random variables.

Definition 50 (Stochastic Process [14, Definition 5.2])**.** Given a set $\mathcal{T} \subset \mathbb{R}$ and a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, a real-valued *stochastic process* (also known as a random process) is a collection of real-valued random variables $\{X(t) : t \in \mathcal{T}\}$. The stochastic process can also be viewed as a map $\Omega \to L^2(\mathcal{T})$.

Definition 51 (Random Field [14, Definition 7.1])**.** Given a set $D \subset \mathbb{R}^d$ and a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, a real-valued *random field* is a collection of real-valued random variables $\{u(\boldsymbol{x}) : \boldsymbol{x} \in D\}$. The random field can also be viewed as a map $\Omega \to L^2(D)$.

Definition 52 (Expected Value)**.** For a continuous random variable X with probability density function (PDF) $f(x)$, the expected value is defined as:

$$\mathbb{E}[X] := \int_{-\infty}^{\infty} x f(x) \, dx.$$

Definition 53 (Covariance [14, Definition 4.14])**.** The covariance of two real-valued random variables X and Y is

$$\operatorname{Cov}(X, Y) := \mathbb{E}[(X - \mu_X)(Y - \mu_Y)] = \mathbb{E}[XY] - \mu_X \mu_Y,$$

where $\mu_X = \mathbb{E}[X]$ and $\mu_Y = \mathbb{E}[Y]$.

Definition 54 (Autocovariance function)**.** The autocovariance function $C(s,t)$ of a stochastic process or random field $\{X(t) : t \in \mathcal{T}\}$ is defined as:

$$C(s,t) := \operatorname{Cov}(X(s), X(t)),$$

for all $s, t \in \mathcal{T}$.

For simplicity we will assume that the expected value will be a constant zero function, i.e., $\mathbb{E}[X] = 0$. Note that if this is not the case, we can instead consider stochastic process $\{Y(t) : t \in \mathcal{T}\}$, where $Y = X - \mathbb{E}[X]$. Then the expected value of Y would be zero.

Definition 55 (Stationary process [14, Definition 6.1])**.** A stochastic process $\{X(t) : t \in \mathcal{T}\}$ is called stationary if its covariance function $C(s,t)$ depends only on the difference $s - t$.

The covariance function of a stationary stochastic process $\{X(t) : t \in \mathcal{T}\}$ can be written as

$$C(s,t) = C(s - t, 0) =: c(s - t),$$

where $c(\tau)$ is known as the stationary covariance function.

Definition 56 (Isotropic Random Field [14, Definition 7.14])**.** A random field $\left\{X(\boldsymbol{x}) : \boldsymbol{x} \in \mathbb{R}^d\right\}$ is isotropic and stationary if its stationary covariance function $c(\boldsymbol{x}) = c^0(r)$, where $r := \|\boldsymbol{x}\|_2$, for a function $c^0 : \mathbb{R}^+ \to \mathbb{R}$ known as the isotropic covariance.

The main focus here will be random fields $X(t)$ with Gaussian distribution, i.e. Gaussian random fields (GRF).

Definition 57 (Gaussian distribution)**.** A random variable X is said to have the Gaussian (or normal) distribution with mean $\mu \in \mathbb{R}$ and variance $\sigma^2 > 0$, if its probability density function (PDF) is given by:

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(x-\mu)^2}{2\sigma^2} \right), \quad x \in \mathbb{R}.$$

We denote this by $X \sim N(\mu, \sigma^2)$.

Definition 58 (Gaussian vector)**.** A random vector $\mathbb{X} \coloneqq (X_1, X_2, \ldots, X_n)$ is said to be a Gaussian vector if there exists $\mu \in \mathbb{R}^n$ and $A \in \mathbb{R}^{n \times m}$ such that $\mathbb{X} = \mu + A\mathbb{Y}$ where $\mathbb{Y}$ is an m-dimensional random vector whose components are independent and have the Gaussian distribution.

Definition 59 (Gaussian Random Field [14, Definition 7.5])**.** A Gaussian random field (GRF) $\{u(\boldsymbol{x}) : \boldsymbol{x} \in D\}$ is a random field such that for any finite set of points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in D$ (where $n \in \mathbb{N}$), the random vector $\boldsymbol{u} = [u(\boldsymbol{x}_1), u(\boldsymbol{x}_2), \ldots, u(\boldsymbol{x}_n)]^T$ follows the multivariate Gaussian (or normal) distribution. Specifically, $\boldsymbol{u} \sim N(\boldsymbol{\mu}, C)$, where the mean vector $\boldsymbol{\mu}$ has components $\mu_i = \mathbb{E}[u(\boldsymbol{x}_i)]$ and the covariance matrix C has entries $C_{ij} = \mathrm{Cov}(u(\boldsymbol{x}_i), u(\boldsymbol{x}_j))$.

3.4 Autocovariance functions

In this section, we will examine some basic autocovariance functions. An original source introducing covariance functions as a tool for describing spacial properties of random field via a family of Matérn covariance functions is [16].

Example 60. Figure 3.1 shows five different autocovariance functions (generated using the implementation in [1]). These include three Matérn covariance functions , each with a different smoothness parameter ν. Also shown are the Squared Exponential (Gaussian) covariance function $C(d) = e^{-\frac{d^2}{2}}$ and the Exponential covariance function $C(d) = e^{-d}$. We note that the Matérn covariance function with $\nu = 0.5$ is equivalent to the exponential covariance function.

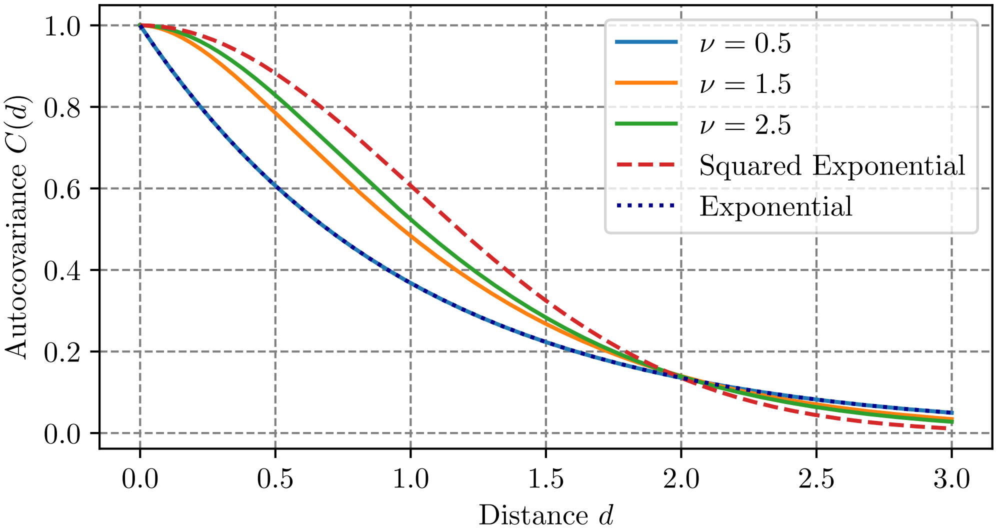

Figure 3.1: Autocovariance Functions

Chapter 4

Karhunen-Loève expansion

This section addresses the Karhunen-Loève (KL) expansion [2, 3], specifically focusing on its application to Isotropic GRF for which we will consider the expected value will be constant zero function, i.e., $\mathbb{E}[X] = 0$. Subsequently, a numerical approximation of the KL expansion is computed using the Galerkin method. Gaussian quadrature techniques are employed for the efficient numerical evaluation of these integrals. The determination of the eigenfunctions and eigenvalues required for the KL expansion inherently corresponds to solving an integral eigenvalue problem, which is conceptually equivalent to the spectral decomposition of the covariance operator associated with the random field. The Galerkin procedure provides a means to discretize this problem, leading to a matrix eigenvalue problem. The main computational part of this method consists of integrals over the specified multi-dimensional domain $\mathcal{T}$.

For more details on KL decomposition and its numerical approximation, we refer the reader to [14, 17]

We are interested in expressing the sample paths of a random field $X(t, \omega) \in L^2(\mathcal{T})$ as a series in an orthonormal basis.

Theorem 61 (Karhunen-Loève)**.** *Let $X(t)$ be a zero mean Gaussian random field, then there exists an orthonormal basis $\{u_j : j \in \mathbb{N}\}$ of $L^2(\mathcal{T})$. Such that*

$$X(t, \omega) = \sum_{j=1}^{\infty} \gamma_j(\omega) \sqrt{\lambda_j} u_j(t), \tag{4.1}$$

where the coefficients γ_j are random variables defined by

$$\gamma_j(\omega) \coloneqq \langle X(t, \omega), u_j(t) \rangle_{L^2(\mathcal{T})}$$

and (λ_j, u_j) are eigenpairs of the autocovariance operator C:

$$(Cu)(x) := \int_{\mathcal{T}} c(x,y)\, u(y)\, dy. \tag{4.2}$$

Remark 62. The random variables γ_j have zero mean, unit variance and are pairwise uncorrelated. Moreover, for GRF they are independent.

Definition 63 (Tensor space)**.** Let us have an N-dimensional space $V_N^x := \operatorname{span}\{\psi_1, \dots, \psi_N\}$ and an M-dimensional space $V_M^y := \operatorname{span}\{\phi_1, \dots, \phi_M\}$. The tensor product space is defined as

$$V_N^x \otimes V_M^y := \operatorname{span}\{\psi_i \phi_j : i = 1, \dots, N, j = 1, \dots, M\}$$

and has dimension NM.

Remark 64. Let $V_{N_i}^{x_i}$, for $i = 1, 2, \dots n$, be a sequence of vector spaces, where each space $V_{N_i}^{x_i}$ has dimension N_i. The tensor product space V_N^x is formed as:

$$V_N^x = V_{N_1}^{x_1} \otimes V_{N_2}^{x_2} \otimes \cdots \otimes V_{N_n}^{x_n}.$$

The dimension of the resulting space V_N^x is $N = \prod_{i=1}^n N_i$.

We want to approximate eigenpairs (λ, u) of C, i.e. find (λ_i, u_i) such

$$(Cu_i)(\boldsymbol{x}) := \int_{\mathcal{T}} c(\boldsymbol{x}, \boldsymbol{y})\, u_i(\boldsymbol{y})\, d\boldsymbol{y} = \lambda_i u_i(\boldsymbol{x}), \quad \forall \boldsymbol{x} \in \mathcal{T}. \tag{4.3}$$

4.1 The Galerkin method for approximation of eigenpairs of autocovariance operator

The Galerkin method is employed to compute approximations of the desired eigenpairs (λ_i, u_i). The Galerkin approach discretizes the underlying operator eigenvalue problem, resulting in a matrix eigenvalue problem whose solutions provide the approximate eigenpairs (λ_i, u_i).

Let us consider a subspace $V_N \subset L^2(\mathcal{T})$ with a basis $\{\psi_j(\boldsymbol{x})\}_{j=0}^N$. We seek an approximation $u_{i,N} \in V_N$ to the eigenfunction u_i, written as a linear combination of the basis functions:

$$u_{i,N} = \sum_{j=0}^{N} \overline{u}_{i,j} \psi_j. \tag{4.4}$$

Next, we substitute the approximation $u_{i,N}$ for u_i into (4.3) and apply the Galerkin method. This involves testing the resulting expression with the basis functions ψ_k in the Galerkin sense, i.e., integrating the residual against ψ_k over the domain $\mathcal{T}$ with respect to $\boldsymbol{x}$. We arrive at the corresponding weak formulation:

$$\sum_{j=0}^{N} \overline{u}_{i,j} \int\limits_{\mathcal{T}} \int\limits_{\mathcal{T}} \psi_k(\boldsymbol{y})\, c(\boldsymbol{x},\boldsymbol{y})\, \psi_j(\boldsymbol{x})\, d\boldsymbol{x} d\boldsymbol{y}. = \lambda_{i,N}^{n} \sum_{j=0}^{N} \overline{u}_{i,j} \int\limits_{\mathcal{T}} \psi_k(\boldsymbol{x})\, \psi_j(\boldsymbol{x})\, d\boldsymbol{x}, \quad \forall k \in \{0,\dots,N\}, \tag{4.5}$$

where $\lambda_{i,N}$ is the approximation of the eigenvalue λ_i. This can be rewritten in a matrix form. Let $\overline{\boldsymbol{u}}_i = [\overline{u}_{i,0},\dots,\overline{u}_{i,N}]^T$ be the vector representation of the Galerkin approximation $u_{i,N}$. Define the matrices A and W with entries:

$$A_{k,j} = \int\limits_{\mathcal{T}} \int\limits_{\mathcal{T}} \psi_k(\boldsymbol{y})\, c(\boldsymbol{x},\boldsymbol{y})\, \psi_j(\boldsymbol{x})\, d\boldsymbol{x} d\boldsymbol{y}$$

and

$$W_{k,j} = \int\limits_{\mathcal{T}} \psi_k(\boldsymbol{x})\, \psi_j(\boldsymbol{x})\, d\boldsymbol{x}.$$

The weak formulation (4.5) then becomes the generalized eigenvalue problem:

$$A\overline{\boldsymbol{u}}_i = \lambda_{i,N} W \overline{\boldsymbol{u}}_i. \tag{4.6}$$

If the kernel $c(\boldsymbol{x},\boldsymbol{y})$ is symmetric and positive semi-definite, the matrix A is symmetric and positive semi-definite. The matrix W (the Gram matrix) is symmetric and positive definite since the basis functions $\{\psi_j\}$ are linearly independent. If the basis functions $\psi_j(\boldsymbol{x})$ are orthonormal (i.e., $W_{kj} = \delta_{kj}$), then W is the identity matrix, leaving us with the standard eigenvalue problem $A\overline{\boldsymbol{u}}_i = \lambda_{i,N}\overline{\boldsymbol{u}}_i$ for the matrix A.

The clear choice for basis functions are the orthonormal polynomials with respect to the domain $\mathcal{T}$. The basis can be then expressed as tensor product of Legendre polynomials, whose construction was thoroughly disseminated in Chapter 2, specifically Remark 27 and Remark 29.

4.2 Numerical experiments

We will construct the matrix A from the generalized eigenvalue problem (4.6). Our aim is to approximate the entries of the matrix A using a series of vector operations, i.e., construct all entries $A_{k,l}$ simultaneously (see [1] for implementation). In this way, we will not recompute the values needed to evaluate the integral numerically multiple times. Note that this approach will calculate all entries, meaning some calculations may be redundant for a symmetric covariance $c(x,y)$. In our code, the calculation involves orthonormal Legendre polynomials $\tilde{\pi}_i, i = 0,\dots,N$, evaluated at quadrature nodes $\tau_i, i = 1,\dots,M$, and the corresponding quadrature weights $w_i, i = 1,\dots,M$.

These vectors will form an $M \times (N+1)$ matrix:

$$\varphi = \begin{bmatrix} w_1\tilde{\pi}_0(\tau_1) & w_2\tilde{\pi}_0(\tau_2) & \cdots & w_M\tilde{\pi}_0(\tau_M) \\ w_1\tilde{\pi}_1(\tau_1) & w_2\tilde{\pi}_1(\tau_2) & \cdots & w_M\tilde{\pi}_1(\tau_M) \\ \vdots & \vdots & \ddots & \vdots \\ w_1\tilde{\pi}_N(\tau_1) & w_2\tilde{\pi}_N(\tau_2) & \cdots & w_M\tilde{\pi}_N(\tau_M) \end{bmatrix}.$$

We also define the $M \times M$ covariance matrix C whose entries are the values of the covariance function evaluated between pairs of quadrature nodes:

$$C = \begin{bmatrix} c\left(\tau_1,\tau_1\right) & c\left(\tau_1,\tau_2\right) & \cdots & c\left(\tau_1,\tau_M\right) \\ c\left(\tau_2,\tau_1\right) & c\left(\tau_2,\tau_2\right) & \cdots & c\left(\tau_2,\tau_M\right) \\ \vdots & \vdots & \ddots & \vdots \\ c\left(\tau_M,\tau_1\right) & c\left(\tau_M,\tau_2\right) & \cdots & c\left(\tau_M,\tau_M\right) \end{bmatrix}, \quad \text{i.e., } C_{ij} = c(\tau_i,\tau_j).$$

The matrix A will then be constructed as:

$$A = \varphi C \varphi^T.$$

Since we are using orthonormal polynomials as basis functions, the matrix W is the identity matrix. The eigenvalues and eigenvectors of matrix A therefore approximate the eigenvalues λ_i and the coefficient vectors $\overline{\boldsymbol{u}}_i$ of the eigenfunctions u_i in Karhunen-Loève expansion respectively.

This approach is also applicable to higher-dimensional fields. One can either:

1. Vectorize: Unroll the domain (quadrature nodes) and the basis function evaluations into long vectors (e.g., using lexicographical ordering). Then, construct the large matrices A and W as in the 1D case and solve the resulting eigenvalue problem.

2. Use Tensor Operations: Treat the operations involved in constructing the matrix A (or applying it to a vector) as tensor contractions. Tools like 'einsum' (e.g., in NumPy) can perform these operations efficiently. 'einsum' takes multiple input tensors and a string describing which dimensions correspond and how they should be contracted or rearranged to produce the desired output tensor. The elements of the tensor A are then computed as:

$$A_{klij} = \sum_{p=1}^{n}\sum_{q=1}^{n}\sum_{r=1}^{n}\sum_{s=1}^{n} \left(\psi_k(x_p)w_p\right)\left(\psi_l(x_q)w_q\right) C_{pqrs} \left(\psi_i(x_r)w_r\right)\left(\psi_j(x_s)w_s\right) \tag{4.7}$$

The next step is to determine an adequate number of quadrature nodes and weights (N) required to compute the entries of the Galerkin matrix A with sufficient accuracy. Since the exact analytical values of the matrix entries $A_{k,l}$ (which involve integrals approximated by quadrature) are generally unknown, a reference value is needed for comparison. We adopt the common approach of assuming that using a significantly larger number of nodes yields a highly accurate result. Therefore, a reference value $A^*_{k,l}$ is computed using a large number of nodes, N_r. The values $A_{k,l}$ computed with fewer nodes ($N < N_r$) are then compared against this reference to assess convergence.

Example 65. This approach is illustrated in Figure 4.1. In this example, matrix entries $A_{k,l}$ were computed from exponential covariance $\mathrm{Cov}(x, y) = \exp\left(-|x - y|\right)$ using N nodes, where N ranged from 10 to 600. These computed values were compared to a reference value $A^*_{k,l}$ computed with $N_r = 5000$ nodes. The figure shows the error, defined as $|A_{k,l} - A^*_{k,l}|$. We may observe that value $A_{5,6}$ is at machine precision the entire time, that is expected due to $A_{5,6}$ being equal to zero.

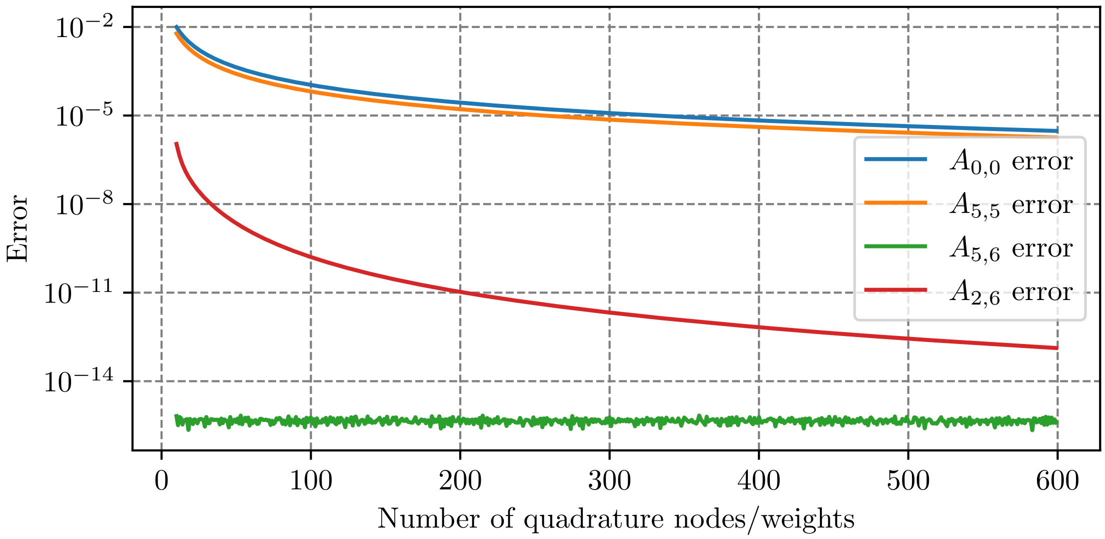

Figure 4.1: Error of entries $A_{k,l}$ obtained from exponential covariance

Example 66. The same approach was used in Figure 4.2. This time, the matrix entries $A_{k,l}$ were computed from the Matérn covariance function using N nodes, where N ranged from 10 to 200. The computed values were compared to a reference value $A^*_{k,l}$ computed with $N_r = 5000$ nodes. Note that the convergence shown in this graph is much faster than that in Figure 4.1. This is because the exponential covariance function is not smooth at $x = y$, whereas the Matérn covariance function (with $\nu = 2.5 > 0.5$) is smooth at $x = y$.

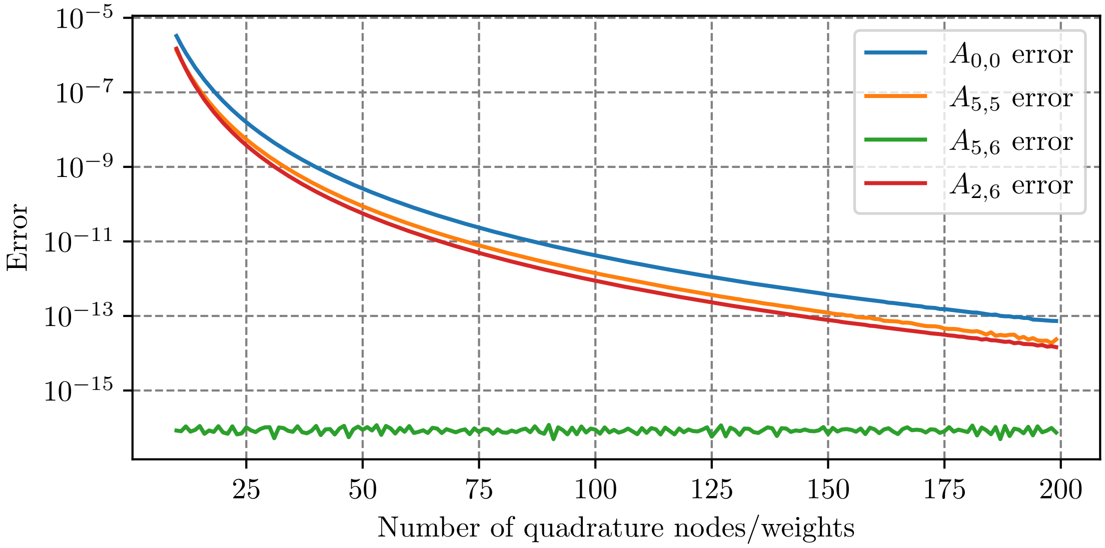

Figure 4.2: Error of entries $A_{k,l}$ obtained from Matérn covariance

We now examine the computed eigenvalues and eigenvectors of the matrix A. Figure 4.3 shows the computed approximate eigenvalues corresponding to different covariance functions; in this case, they were calculated using 61 orthonormal basis functions.

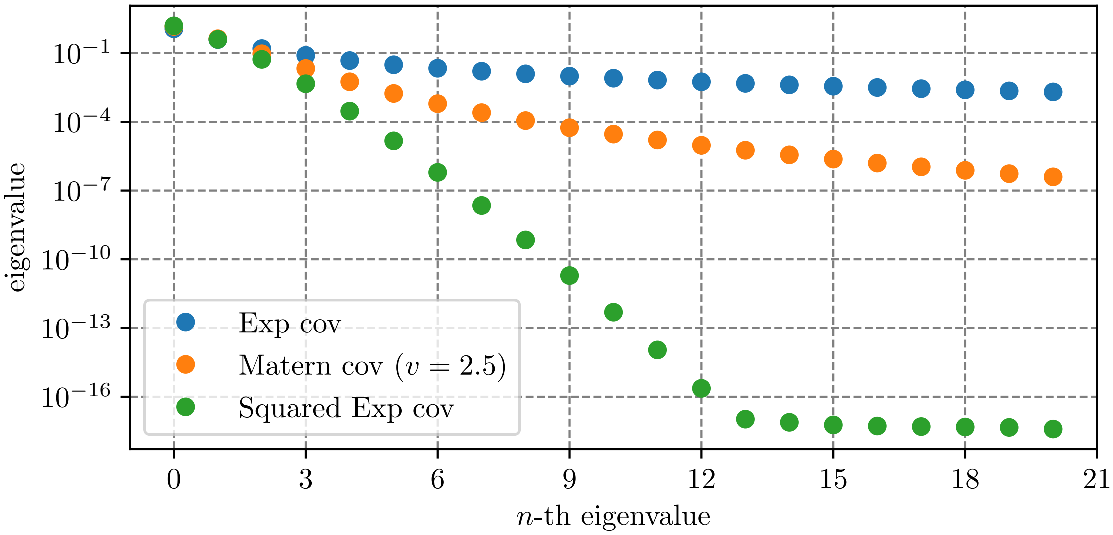

Figure 4.3: Approximate 1D eigenvalues from different covariance functions

Figure 4.4 shows the first six eigenfunctions corresponding to the exponential covariance function $\text{Cov}(x, y) = \exp(-|x - y|)$ multiplied by the square root of corresponding eigenvalue, i.e. $u_i(x)\sqrt{\lambda_i}$. In a same way Figure 4.5 shows $u_i(x)\sqrt{\lambda_i}$ approximations for squared exponential covariance and Figure 4.6 shows $u_i(x)\sqrt{\lambda_i}$ approximations for Matérn covariance.

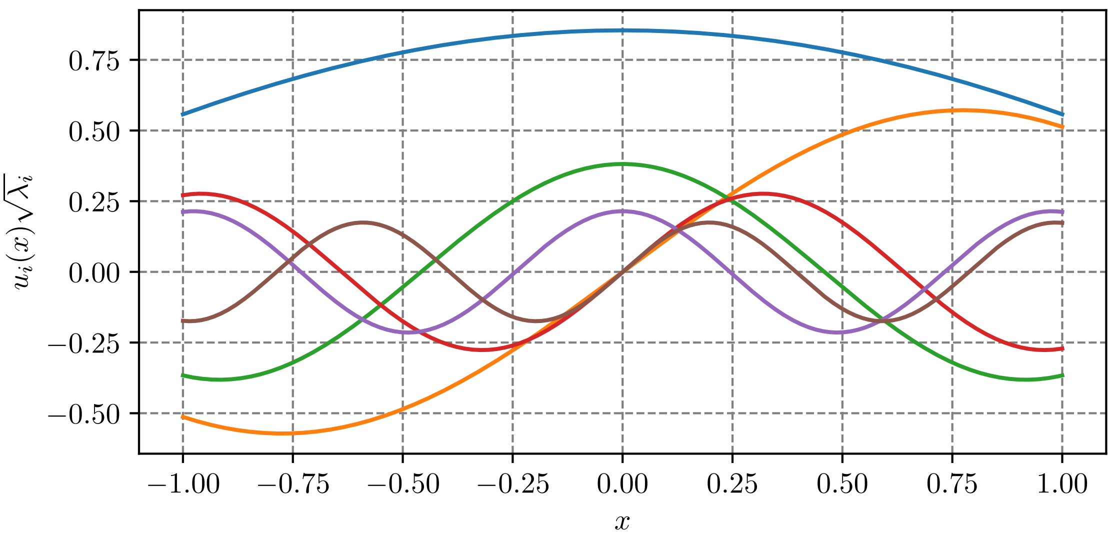

Figure 4.4: Functions $u_i(x)\sqrt{\lambda_i}$ used in KL for exponential covariance (4.1) in 1D

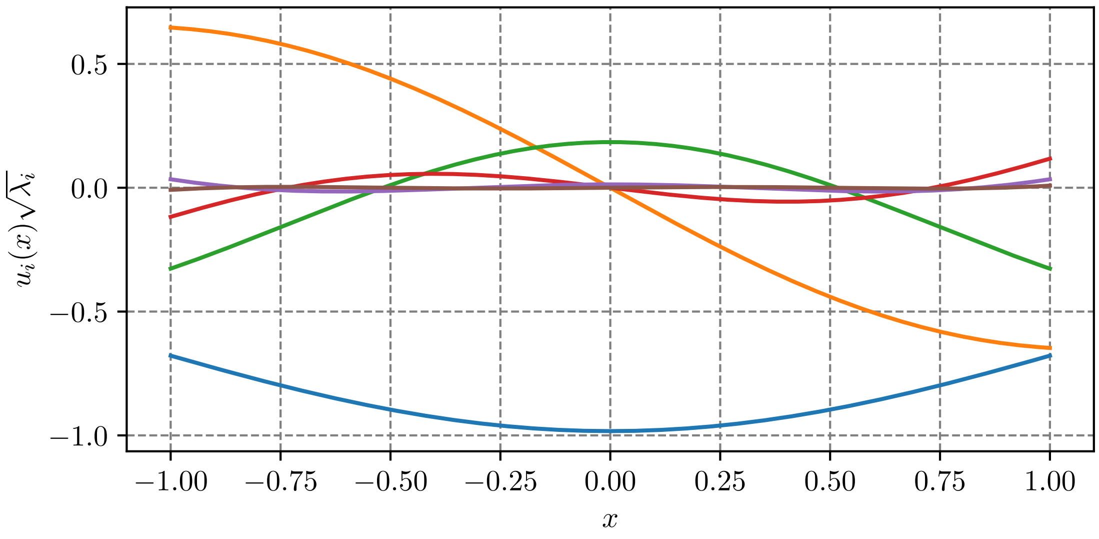

Figure 4.5: Functions $u_i(x)\sqrt{\lambda_i}$ used in KL for squared exponential covariance (4.1) in 1D

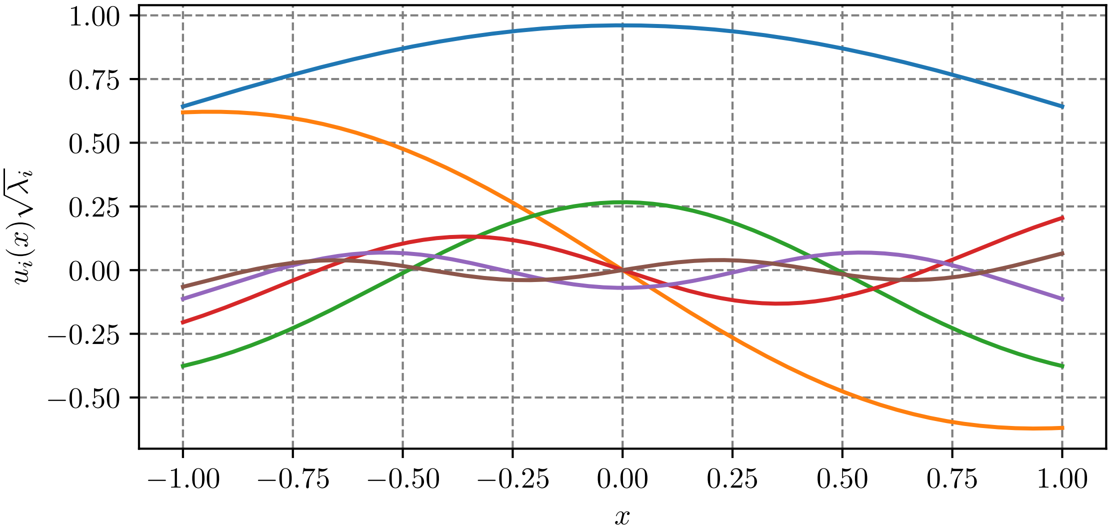

Figure 4.6: Functions $u_i(x)\sqrt{\lambda_i}$ used in KL for Matérn covariance (4.1) in 1D

Figures 4.7, 4.8 and 4.9 each illustrate three sampled realizations generated using the Karhunen-Loève (KL) expansion with different covariance functions. Figure 4.7 used the exponential covariance function, Figure 4.8 used the squared exponential covariance function and Figure 4.9 used the Matérn covariance function with parameter $v = 2.5$. Note that sampling the realizations is computationally inexpensive, as it involves multiplying the eigenfunctions by the square root of the eigenvalues and by samples from a standard Gaussian distribution.

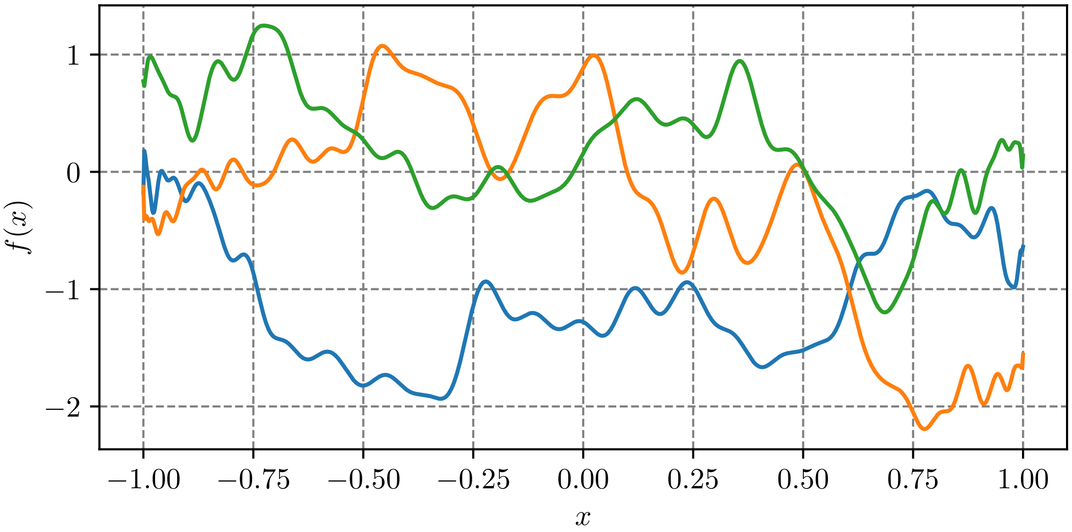

Figure 4.7: Sample realizations of a 1D random field with a exponential covariance function

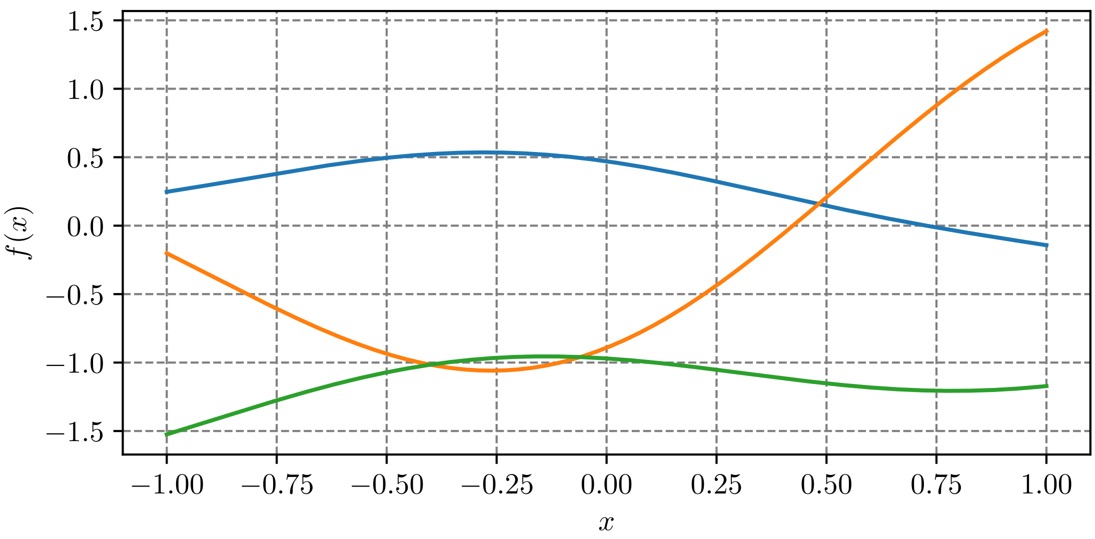

Figure 4.8: Sample realizations of a 1D random field with a squared exponential covariance function

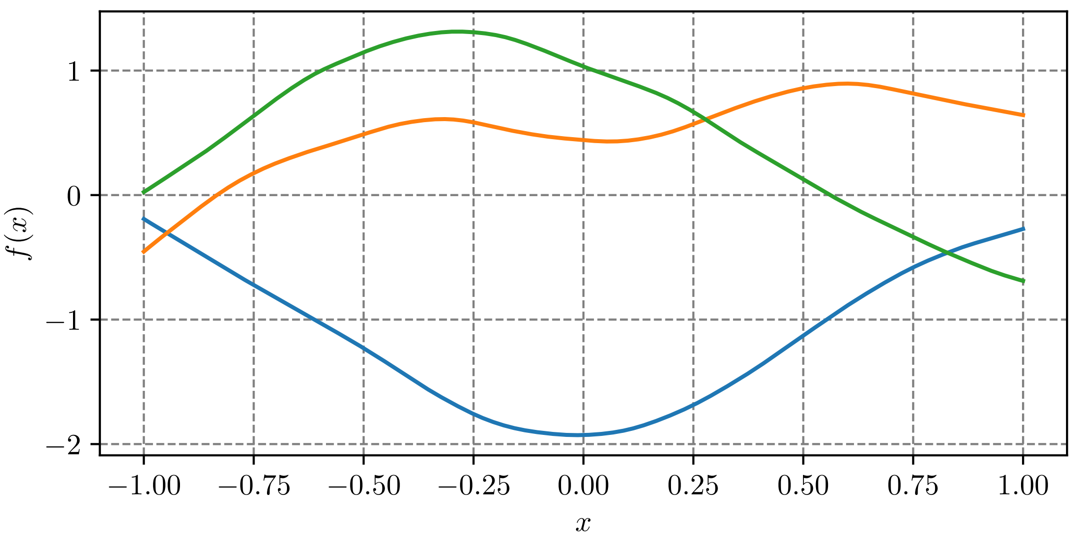

Figure 4.9: Sample realizations of a 1D random field with a Matérn covariance function

The accuracy of the approximated eigenpairs $\left(\tilde{\lambda}_i, \tilde{u}_i\right)$ obtained from the Galerkin method can be quantified by examining the residual error. This residual measures how closely the approximate solution satisfies the original integral eigenvalue problem (4.3). The magnitude of this error is typically measured using the L^2-norm of the residual function $R_i(x) = \int_{\mathcal{T}} c\left(x, y\right) \tilde{u}_i\left(y\right)\, dy - \tilde{\lambda}_i \tilde{u}_i\left(x\right)$, defined as:

$$\|R_i\|_{L^2} = \left\| \int_{\mathcal{T}} c\left(x,y\right) \tilde{u}_i\left(y\right)\, dy - \tilde{\lambda}_i \tilde{u}_i\left(x\right) \right\|_{L^2} = \left(\int_{\mathcal{T}} \left(\int_{\mathcal{T}} c\left(x,y\right) \tilde{u}_i\left(y\right)\, dy - \tilde{\lambda}_i \tilde{u}_i\left(x\right) \right)^2 dx \right)^{1/2} .$$

In Figure 4.10, we see the residual for the first five approximate eigenpairs, computed for the exponential covariance function, for increasing number of basis polynomials. Similarly, Figure (4.11) presents the corresponding residual results for the squared exponential covariance function. The residual behavior for the Matérn covariance function is illustrated in Figure 4.12. We observe that the residual decreases substantially only for either the even- or odd-indexed eigenpairs at each step, in an alternating fashion. This is because the basis polynomials being added alternate between even and odd degrees, and adding a polynomial of a certain parity primarily refines the approximations of the eigenpairs with the corresponding parity.

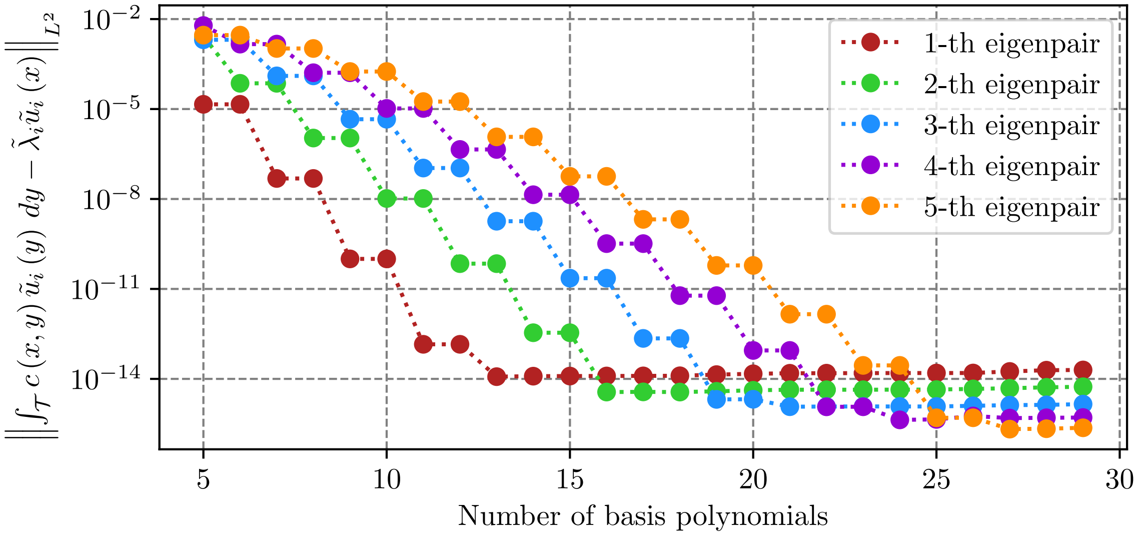

Figure 4.10: L^2-norm of the residuum of eigenpairs for 1D exponential covariance

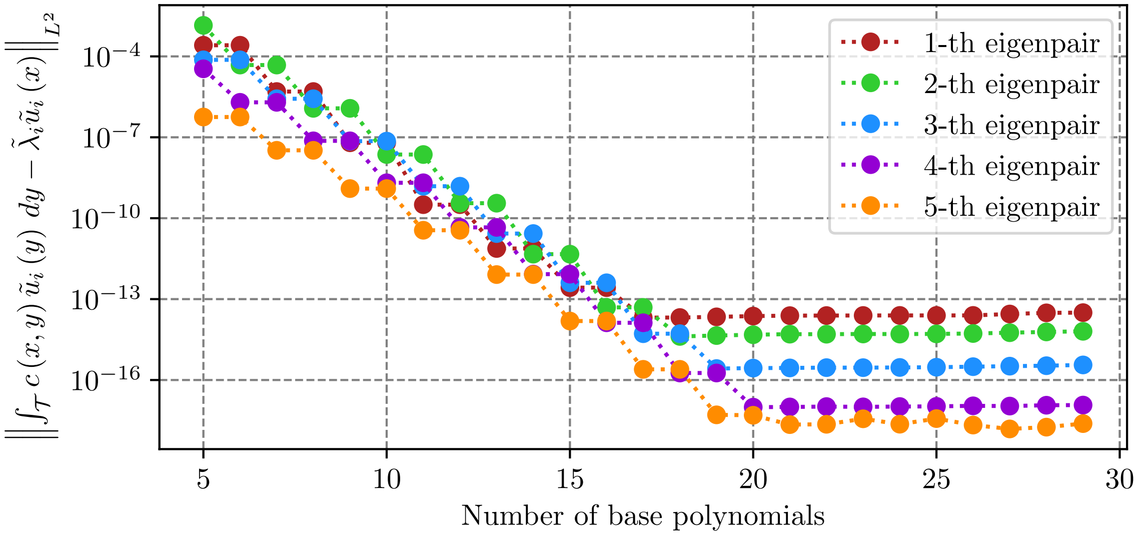

Figure 4.11: L^2-norm of the residuum of eigenpairs for 1D squared exponential covariance

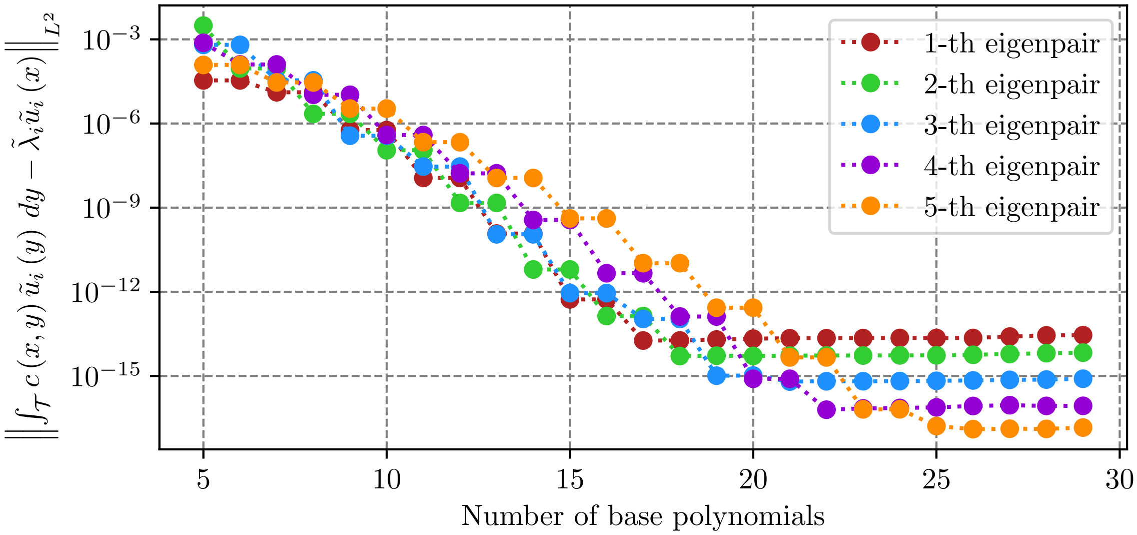

Figure 4.12: L^2-norm of the residuum of eigenpairs for 1D Matérn covariance

The analysis is now extended to two-dimensional random fields defined on the square domain $\mathcal{T} = \langle -1, 1\rangle \times \langle -1, 1\rangle$. We examine the Karhunen-Loève (KL) expansion components and resulting field realizations for two different isotropic covariance models. Those covariance models are the exponential covariance function, $\mathrm{Cov}(\boldsymbol{x}, \boldsymbol{y}) = \exp\left(-\|\boldsymbol{x} - \boldsymbol{y}\|\right)$, and squared exponential covariance function, $\mathrm{Cov}(\boldsymbol{x}, \boldsymbol{y}) = \exp\left(-\|\boldsymbol{x} - \boldsymbol{y}\|^2/2\right)$. All visualizations presented in this section correspond to this domain $\mathcal{T}$. Firstly, we examine the eigenvalues for these covariance functions, shown in Figure 4.13.

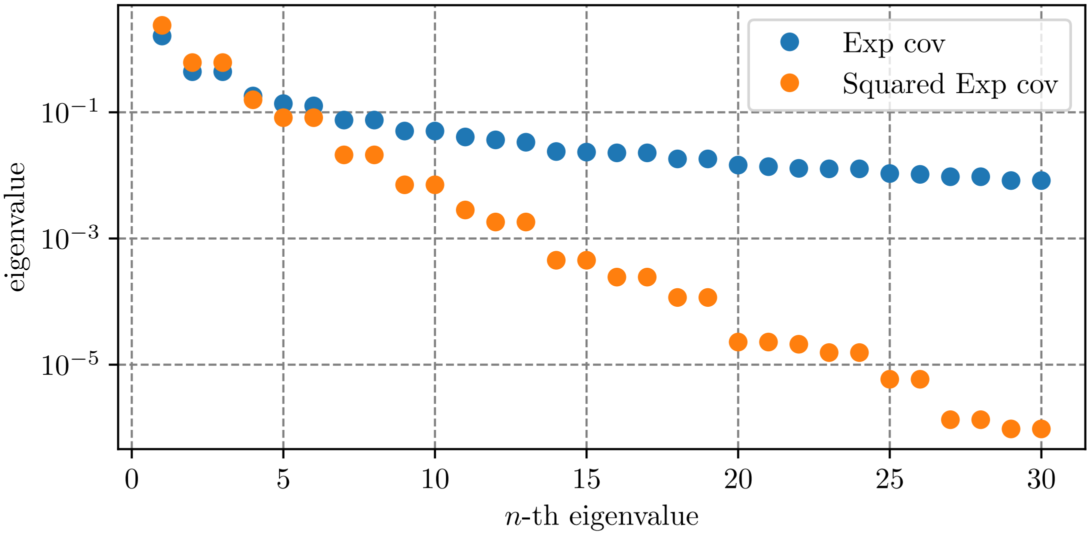

Figure 4.13: Eigenvalues for the different covariance functions in 2D

Figure 4.14 displays the first six computed approximate eigenfunctions, $\tilde{u}_i(\boldsymbol{x})$, scaled by the square root of the corresponding eigenvalues, $\sqrt{\tilde{\lambda}_i}$, derived from the exponential covariance function on $\mathcal{T}$. Similarly, Figure 4.15 shows the first six approximate eigenfunctions $\tilde{u}_i(\boldsymbol{x})$ scaled by $\sqrt{\tilde{\lambda}_i}$, derived from the squared exponential covariance function on the same domain. A notable characteristic observed in both sets (Figures 4.14 and 4.15) is their distinct "symmetry", reflecting the isotropic nature of the underlying covariance functions.

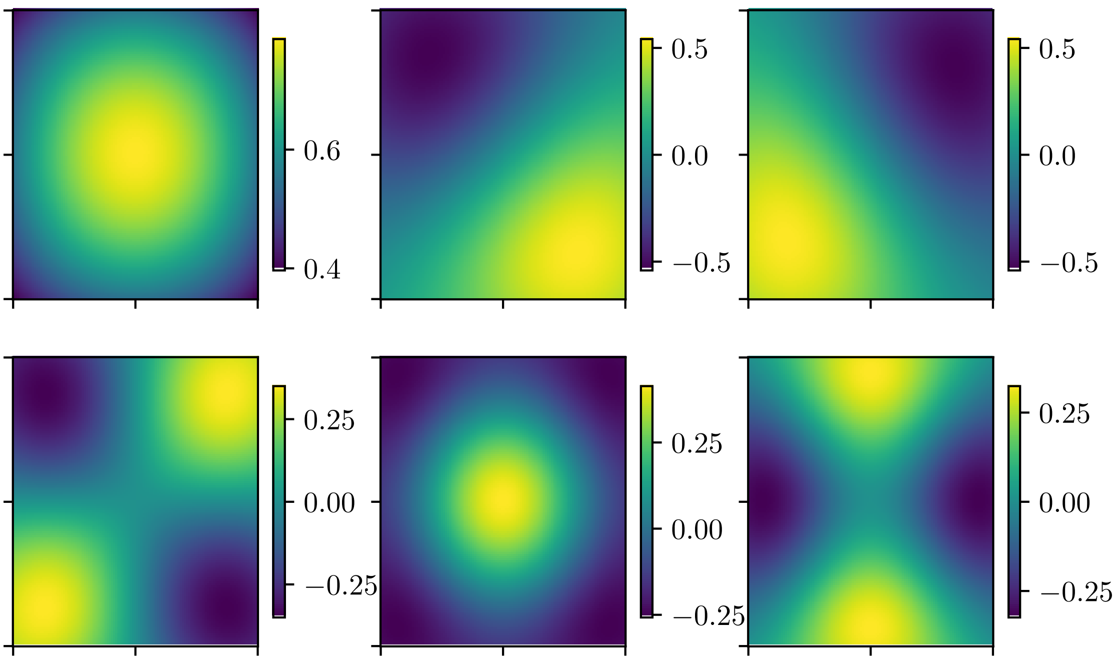

Figure 4.14: Approximate 2D functions $\tilde{u}_i(\boldsymbol{x})\sqrt{\tilde{\lambda}_i}$ for the exponential covariance function, defined on the domain $\langle -1, 1\rangle \times \langle -1, 1\rangle$

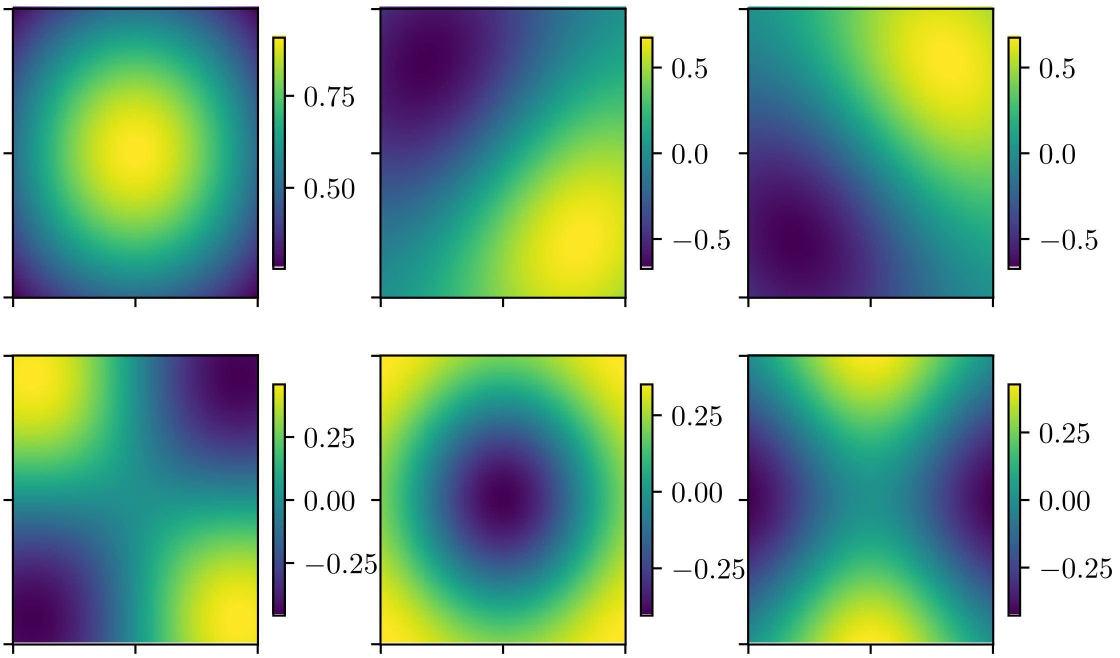

Figure 4.15: Approximate 2D functions $\tilde{u}_j(\boldsymbol{x})\sqrt{\tilde{\lambda}_i}$ for the squared exponential covariance function, defined on the domain $\langle -1, 1\rangle \times \langle -1, 1\rangle$

Next, plots of sample fields generated using these KL expansions are shown. Figure 4.16 illustrates six sample realizations of the two-dimensional random field modeled with the exponential covariance function. Figure 4.17 provides corresponding sample realizations for the field modeled with the squared exponential covariance function. These plots offer visual examples of the texture and spatial structure characteristic of random fields resulting from these respective covariance models over the domain $\mathcal{T}$. Comparing the two sets of samples reveals that the sampled realizations from the squared exponential covariance function appear much smoother than those from the exponential covariance function. That is because the squared exponential maintains high correlation locally much more strongly than the exponential. Note that sampling a 2D realization is performed simply in our code. It involves multiplying an eigenfunction, the square root of the corresponding eigenvalue, and a sample from a standard normal distribution.

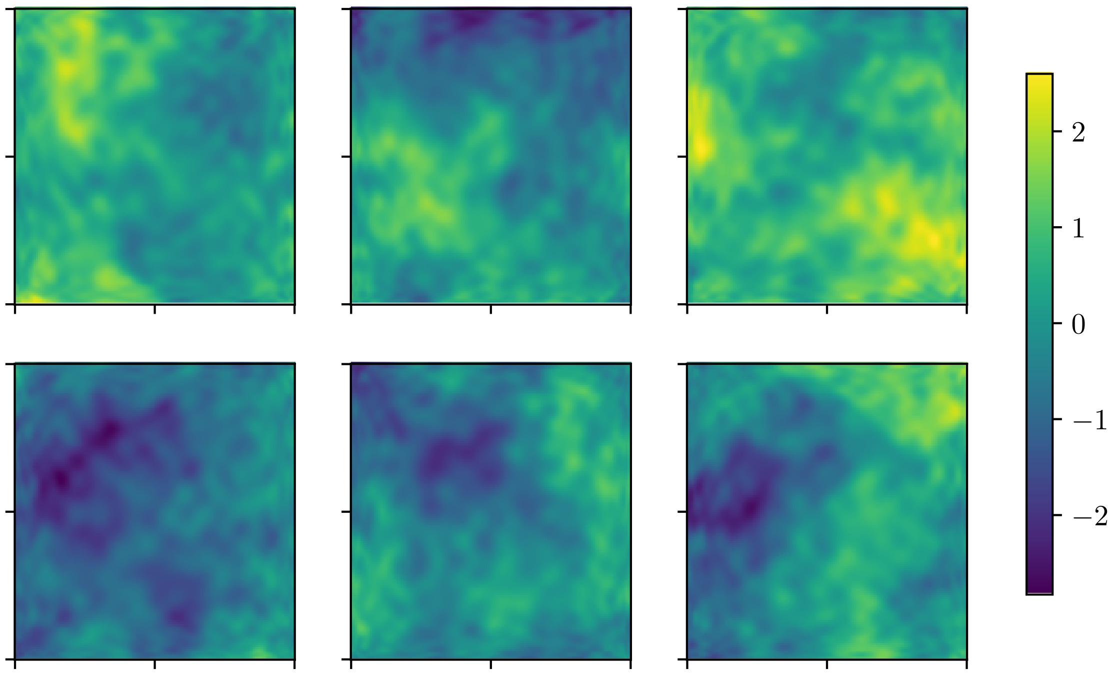

Figure 4.16: Sample realizations of a 2D random field with an exponential covariance function, defined on the domain $\langle -1, 1\rangle \times \langle -1, 1\rangle$

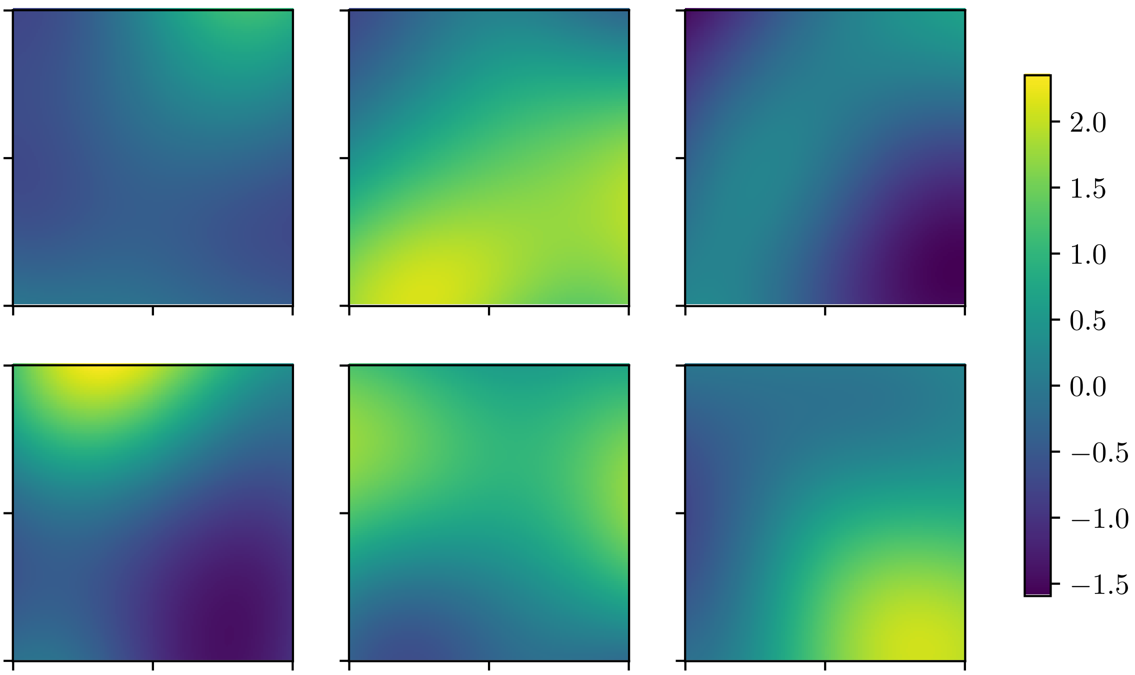

Figure 4.17: Sample realizations of a 2D random field with a squared exponential covariance function, defined on the domain $\langle -1, 1\rangle \times \langle -1, 1\rangle$

Chapter 5

Conclusion

This thesis aimed to implement a numerical method for computing the Karhunen-Loève (KL) expansion of a random field. The method combined the theory of orthogonal polynomials, Gaussian quadrature, and the Galerkin technique to solve the integral eigenvalue problem associated with the random field's autocovariance function.

We began in Chapter 2 by establishing the necessary mathematical tools related to orthogonal polynomials, specifically Legendre polynomials. This included their definition via weighted inner products, their construction using the three-term recurrence relation, the connection to Jacobi matrices, and the derivation of Gaussian quadrature rules using the Golub-Welsch algorithm. The details of modifying these techniques for application on any finite interval $\langle a, b \rangle$ was also detailed. At the end of Chapter 2 provided numerical validation of these concepts, demonstrating the generation of polynomials and the efficiency and convergence properties of Gaussian quadrature for various integrands.

Chapter 3 provided the necessary background in probability theory, explaining terms such as L^2 space, probability spaces, random variables, random fields, and autocovariance functions, with a focus on Gaussian random fields (GRF) which are commonly used in applications.

The core objective was addressed in Chapter 4, where the Karhunen-Loève theorem was presented. We then detailed the Galerkin method for approximating the KL eigenpairs (λ_i, u_i). This method utilizes the orthonormal Legendre polynomials from Chapter 2 as basis functions and employs Gaussian quadrature rules, also from Chapter 2, for the efficient calculation of the integrals needed to form the Galerkin matrix system. The numerical experiments in this chapter successfully demonstrated the computation of approximate KL eigenvalues and eigenfunctions for selected covariance functions and showed the convergence of the method by analyzing the residual error.

In terms of contribution, a significant part of this thesis, particularly Chapters 2 and 3, involved the compilation and concise presentation of established mathematical theory from existing literature [5, 14]. These sections aimed to gather the necessary background information in a structured and accessible manner.

The key practical outcome of this work lies in the implementation and integration of these theoretical components into a working computational pipeline in (see [1]). This task involved creating and testing the code (as evidenced by the results in Chapters 2 and 4) to:

- Generate Legendre polynomials and their recurrence coefficients.
- Compute Gaussian quadrature nodes and weights using the Golub-Welsch algorithm.
- Assemble the Galerkin matrices using Gaussian quadrature to evaluate the required integrals involving the polynomial basis and the covariance kernel.
- Solve the resulting matrix eigenvalue problem to obtain approximate KL eigenpairs.
- Visualize and analyze the computed KL components and their accuracy.

Bringing these distinct mathematical tools together to successfully approximate the Karhunen-Loève expansion and demonstrating the process through concrete numerical examples constitutes the core practical achievement of this thesis.

Overall, this thesis successfully demonstrated the effectiveness of using orthogonal polynomials and Gaussian quadrature within a Galerkin framework for the numerical approximation of the Karhunen-Loève expansion. It provides a practical guide to the underlying theory and its implementation, confirming the utility of these combined techniques for computationally representing stochastic processes.

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