

GENERALIZED OPTIMAL THRESHOLD FACTORS AND STRUCTURE-PRESERVING EXPONENTIAL INTEGRATORS

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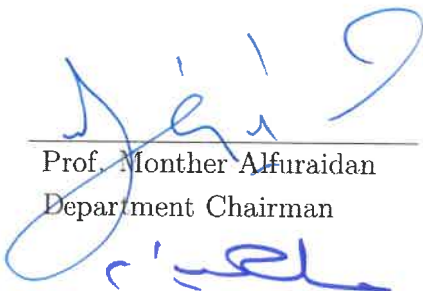
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Dedication
To my father, Nasser Al-Tamimi
and my mother, Aysha Al-Tamimi

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DISSERTATION ABSTRACT

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TITLE OF STUDY: Generalized Optimal Threshold Factors and Structure-Preserving Exponential Integrators

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This thesis develops a comprehensive framework for designing high-order exponential integrator schemes that preserve key structural properties - positivity and contractivity - in the numerical integration of differential equations. The central task is formulated as the identification, among all polynomials of a given degree with prescribed successive derivatives at the origin up to a given order, the one with the largest interval of absolute monotonicity on the negative axis. The length of this maximal interval is referred to as the generalized optimal threshold factor, and the corresponding polynomial is termed the optimal threshold polynomial.

To address this question, we introduce a new class of discrete measures whose associated orthogonal polynomials and their zeros offer a complete framework for analyzing optimal threshold factors and the corresponding polynomials. In particular, these measures allow for the derivation of sharp bounds on the optimal threshold fac-

tors using Gaussian quadrature. Furthermore, an efficient algorithm based on adaptive Christoffel spectral transform is developed to compute optimal threshold factors and their associated polynomials in the high-degree regime.

Building on this foundation, we construct structure-preserving exponential integrator schemes with high-order of accuracy. These schemes are applied to semi-discretized partial differential equations, with numerical experiments confirming theoretical bounds and demonstrating reliable behavior under step-size constraints.

Overall, this work delivers a practical and theoretically grounded framework for designing structure-preserving exponential integrators suitable for the robust simulation of physical systems.

ملخص الرسالة

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عنوان الدراسة:

تعميم العوامل الحدية المثالية و التكاملات الأساسية المحافظة على البنى

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تُقدّم هذه الرسالة إطاراً شاملاً لتصميم مخططات تكامل أُسية عالية الرتبة تحافظ على الخصائص البنوية الأساسية — مثل الإيجابية والانكماش — في التكامل العددي للمعادلات التفاضلية. وتتمثل المهمة الرئيسة في تحديد، من بين جميع كثيرات الحدود ذات درجة معينة ومشتقات متتالية محددة عند الأصل حتى رتبة معينة، تلك التي تمتلك أطول مجال للرتابة المطلقة على المحور السالب. يُطلق على طول هذا المجال الأعظمي اسم العامل الحديّ الأمثل المعمم، بينما تُعرف كثيرة الحدود المقابلة بـ كثيرة الحدود الحديّة المثلى.

لمعالجة هذه المسألة، نقدّم صنفًا جديدًا من المقاييس المنفصلة، التي تتيح كثيراتها المتعامدة وجذورها إطارًا تحليليًا متكاملًا لدراسة العوامل الحديّة المثلى وكثيرات الحدود المرتبطة بها. وتُمكن هذه المقاييس من اشتقاق حدود دقيقة للعوامل الحديّة المثلى باستخدام قاعدة التوزيع الغاوسي. علاوة على ذلك، تم تطوير خوارزمية فعالة تعتمد على تحويل كريستوفل الطيفي التكيفي لحساب العوامل الحديّة المثلى وكثيرات الحدود المرتبطة بها في الحالة ذات الدرجة العالية.

استنادًا إلى هذا الأساس، نقوم ببناء مخططات تكامل أُسية محافظة على البنية وتحقق دقة عالية. وتُطبّق هذه المخططات على معادلات تفاضلية جزئية بعد التقطيع المكاني، حيث تؤكد التجارب العددية صحة الحدود النظرية وتُظهر سلوكًا موثوقًا به ضمن قيود على حجم الخطوة الزمنية. بوجه عام، توفّر هذه الرسالة إطارًا عمليًا ومدعومًا نظريًا لتصميم مخططات تكامل أُسية محافظة على البنية، مناسبة لمحاكاة موثوقة للأنظمة الفيزيائية.

CHAPTER 1

INTRODUCTION

In the field of geometric integration, the effectiveness of a numerical method is determined not only by its accuracy but also by its ability to preserve the intrinsic structural properties of the underlying problem. This is particularly important in areas such as computational biology, physics, and chemistry, where state variables often represent non-negative, dissipative, or conservative quantities [1], [2], [3], [4], [5], [6].

A central challenge in designing unconditionally structure-preserving numerical schemes for differential equations lies in overcoming the so-called order barrier [7], [8], [9], [10]. Thus, developing high-order structure-preserving methods should focus on maximizing the permissible step size while maintaining the desired solution properties. This thesis aims to establish a comprehensive framework for high-order exponential integrator schemes that preserve essential structural characteristics. The focus is on deriving optimal positivity-preserving high-order exponential integrators for non-homogeneous linear problems using a generalized notion of optimal threshold factors associated with absolutely monotonic functions. Applications to partial differential equations will be examined in detail.

The initial-value problem

$$\frac{du}{dt} = Au(t) + f(t), \quad u(0) = u_0, \quad u_0 \in \mathbb{R}^s, \quad (1.1)$$

where A is a square matrix of order s and $f : \mathbb{R} \rightarrow \mathbb{R}^s$, is often encountered in the semi-discretisation of partial differential equations [11]. The solution to (1.1) can be expressed as

$$u(t) = e^{At}u_0 + \int_0^t e^{(t-\tau)A}f(\tau) d\tau. \quad (1.2)$$

Many explicit numerical methods for solving (1.1), such as the exponential integrators [12], provide schemes of the form

$$u_{n+1} = r_0(hA)u_n + h \sum_{i=1}^s r_i(hA)f(t_n + c_ih), \quad (1.3)$$

where h is the step-size, u_n is an approximation of $u(nh)$, $c_1, \dots, c_p$, are collocation points in the interval $[0, 1]$ and $r_0, r_1, \dots, r_s$, are rational functions. Achieving high local accuracy in the numerical scheme (1.3) requires specific conditions on the rational functions and collocation points [13]. These conditions are realized by specifying the derivatives of each rational function at zero up to a defined order. For instance, if $f \equiv 0$, the scheme is given by

$$u_{n+1} = r_0(hA)u_n, \quad (1.4)$$

and a local accuracy of order p of the scheme is translated to

$$r_0(z) = e^z + O(z^{p+1}) \quad \text{as } z \longrightarrow 0.$$

The initial-value problem (1.1) is said to *preserves positivity* if, given non-negative initial data ($u_0 \geq 0$) and a non-negative forcing term ($f(t) \geq 0$ for $t \geq 0$), the solution $u(t)$ remains non-negative for all $t \geq 0$. (Inequalities here and everywhere else are interpreted componentwise). It is established in [14] that this positivity preservation occurs if and only if the matrix A is Metzler (i.e., its off-diagonal elements are non-negative). Likewise, the numerical scheme (1.3) is said to preserve positivity if $u_n \geq 0$ for all $n \geq 0$. For the scheme to preserve positivity for any Metzler matrix A , it is necessary and sufficient that $r_j(hA) \geq 0$ for all $j = 0, 1, \dots, s$. It is shown in [14] that no numerical scheme of the form (1.3) can achieve an order of accuracy higher than 2, while unconditionally preserving positivity. Moreover, the schemes (1.3) preserve positivity for any step-size h such that

$$h \leq \frac{\min(R(r_0), R(r_1), \dots, R(r_s))}{\sigma(A)} \quad \text{where } \sigma(A) = \max_{a_{ii} < 0} |a_{ii}|, \quad (1.5)$$

and $R(r_j)$ stands for the *threshold factor* of the function r_j , i.e.; the largest real number R for which the function r_j is *absolutely monotonic* over the interval $[-R, 0]$. Analogue studies [15] have explored contractivity-preserving schemes of the form (1.3). For practical applications, it is crucial to allow flexibility in step-size selection while maintaining both positivity preservation and high accuracy of the numerical schemes.

Therefore, one should aim for functions r_j with the largest threshold factors while still achieving the required accuracy. In the case the functions $r_j, j = 0, 1, \dots, s$ are polynomial functions, the order p requirement for the scheme (1.3) is equivalent to

$$r_0(z) - e^z = O(z^{p+1}), \quad r_i(z) - b_i(z) = O(z^p), \quad \text{as } z \rightarrow 0,$$

where

$$b_i(z) = \int_0^1 e^{(1-\theta)z} \ell_i(\theta) d\theta, \quad i = 1, 2, \dots, s,$$

where ℓ_i is the i -em Lagrange polynomial based on the collocation points. Since the successive derivatives at the origin of each polynomial r_i depend on the collocation points, the central task in designing optimal structure-preserving schemes is to solve the following problem.

• **Central Problem**

Given a sequence of positive real numbers $\Lambda_{p+1} = (\lambda_0, \lambda_1, \dots, \lambda_p)$ and an integer $m \geq p$, find a polynomial F of degree m with the largest interval of absolute monotonicity of the form $[-R, 0]$ and such that $F^{(k)}(0) = \lambda_k$ for $k = 0, 1, \dots, p$.

We note the similarity between our central problem and the following Bernstein problem.

• **Bernstein Problem**

*Given a sequence of positive real numbers $\Lambda_{p+1} = (\lambda_0, \lambda_1, \dots, \lambda_p)$, find the **Bernstein constant**, $R_\infty(\Lambda_{p+1})$, defined as the supremum of positive real number R such that there exists a smooth function F absolutely monotonic over the interval $(-R, 0]$ and such that $F^{(k)}(0) = \lambda_k$ for $k = 0, 1, \dots, p$.*

Our work will shed light into Bernstein problem as it can be viewed as a finite version of it.

In Chapter 2, we show that for any number of stages m , there exists a unique polynomial $\Phi_m(\Lambda_{p+1})$ and a real number $R_m(\Lambda_{p+1})$ that together solve our central problem. We shall term $R_m(\Lambda_{p+1})$ the *optimal threshold factor* and $\Phi_m(\Lambda_{p+1})$ the *optimal threshold polynomial* associated with the sequence Λ_{p+1} . We provide explicit expressions for small values of p and develop an algorithm, based on blossoming theory, for their computation.

In Chapter 3, we introduce a new discrete measure for which the zeros of their associated discrete orthogonal polynomial provide significant insights into both our main problem and the Bernstein problem. The new introduced discrete orthogonal polynomials generalize several classical families, including the Poisson-Charlier, Meixner, and Krawtchouk polynomials. We derive their corresponding three-term recurrence relation and elucidate their connection to our central task.

In Chapter 4, we employ the newly introduced discrete orthogonal polynomials to derive sharp bounds for the optimal threshold factor. The upper bound is established by comparing the nodes of positive quadrature formulas with integer nodes to those of the Gaussian quadrature associated with the discrete measure. This leads to precise bounds for the optimal threshold factors for generalized Poisson-Charlier sequences in terms of the smallest zero of generalized Laguerre polynomials; and for Meixner sequences in terms of the smallest zero of non-standard Jacobi polynomials.

The complexity of the algorithm for computing the optimal threshold factors introduced in Chapter 2 grows exponentially with the number of stages m and the order p .

To compute these factors for large values of m and p , we study the spectral Christoffel transformations of our newly introduced discrete measure in Chapter 5. This leads to a highly efficient and stable algorithm for computing the optimal threshold factors with the particularity that its complexity depends only on the order p .

In Chapter 6, we begin by reviewing exponential integrator methods, followed by a discussion of the necessary and sufficient conditions for these schemes to preserve positivity. Building on the results from the preceding sections, we derive explicit formulas for low-order optimal positivity-preserving exponential integrators. Particular emphasis is placed on optimal schemes whose collocation points coincide with the zeros of classical orthogonal polynomials.

Chapter 7 presents numerical tests and validations for partial differential equations, focusing on two representative models a transport equation and a solar thermal storage system.

1.1 Literature Review

Structure-preserving numerical methods have become an essential subfield in the numerical approximation of ordinary differential equations (ODE) and partial differential equations (PDE), where maintaining critical qualitative characteristics, such as positivity, monotonicity, and contractivity, at the discrete level is vital for stability and physical fidelity [16], [17], [18], [19], [20], [21], [22]. These methods are not only mathematically elegant but practically necessary in simulations involving long-time integration or stiff dynamics.

The theory has seen substantial developments recently; we refer to [23] for a comprehensive review. These methods have been extensively studied and applied across various disciplines, including computational biology, chemistry, and scientific computing [24], [25], [2], [26], [8], [27], [28], [29], where preserving structural properties is crucial. Despite these advancements, determining the optimal step-size that ensures stability while maintaining computational efficiency remains a major challenge, motivating the development of novel schemes and techniques [30], [31].

Bernstein’s foundational work [32] laid the theoretical groundwork by introducing absolutely monotonic functions, which serve as a key mathematical framework for stability and positivity analysis. While Bolley and Crouzeix [14] leveraged Bernstein’s theory to derive limits on unconditional positivity, Kraaijevanger’s work [33] independently introduced criteria for positivity preservation based on polynomial approximations to the exponential function.

Initially, Kraaijevanger [33] explored polynomial approximations to the exponential function and introduced fundamental results for positivity-preserving schemes using absolute monotonicity as a criterion. In a later and distinct contribution, he developed a rigorous contractivity framework for Runge–Kutta methods [34], establishing a deep connection between absolute monotonicity and contractivity in solving nonlinear differential equations. Contractivity generalizes the concept of monotonicity by ensuring that the numerical solution remains bounded in norm relative to the exact solution, even under nonlinear dynamics. This theory extended Spijker’s earlier sufficient condition and unified the analysis of stability and monotonicity in numerical schemes. The link between contractivity and positivity-preserving properties was

further clarified by Horváth [35].

Building on this foundation, Ketcheson [19] designed efficient algorithms that drastically reduced the computational cost of determining optimal monotonicity-preserving coefficients. While early methods required days to compute coefficients for moderate orders, Ketcheson’s improvements enabled the practical generation of high-order methods.

Further advancing this area, Ait-Haddou [36] proposed an innovative approach using adaptive spectral transformations of Poisson–Charlier measures. A major advantage of his method is that its complexity depends solely on the method’s order, not on the number of stages, enabling significantly improved efficiency. His formulation, inspired by Bernstein’s theory, introduced a geometric strategy for constructing absolutely monotonic polynomials with integer exponents occurring in consecutive pairs. Unlike previous approaches that rely on nonlinear optimization, Ait-Haddou’s method achieves optimality through a purely algebraic construction rooted in orthogonal polynomial quadrature and geometric criteria inspired by Bernstein’s theory. This yields highly structured algorithms that efficiently generate optimal positivity- and contractivity-preserving coefficients.

The theoretical and computational basis of these developments draws heavily from classical results in orthogonal polynomials and numerical integration. Karlin and Szegő [37] analyzed positivity via determinant structures, while Ramshaw [38] introduced geometric constructions essential for polynomial representations. Gallant [39] contributed a practical implementation of Christoffel’s theorem, which remains fundamental in transforming orthogonal systems in computational settings—especially in

the context of Ait-Haddou’s spectral algorithms.

Finally, the practical utility of these advances is best illustrated by their application to exponential integrators. Originally introduced by Hersch [40], exponential integrators were developed further by Hochbruck and Ostermann [12], who emphasized their value in solving stiff PDEs. These methods integrate stiff linear parts analytically, improving stability and accuracy. Cox and Matthews [41] proposed exponential time-differencing (ETD) schemes that efficiently apply this principle. Higham [42] later provided an extensive treatment of matrix function algorithms—such as Padé approximants and Schur decompositions—that underpin the practical implementation of such schemes. These methods offer a natural testbed for the positivity- and contractivity-preserving integrators developed in this work, especially in the context of stiff problems where structure-preservation is critical to long-time accuracy.

1.2 Aims and Objectives

The goal of this thesis is threefold. First, to develop exponential time-differencing methods of prescribed order for non-homogeneous problems that preserve the positivity property of the underlying equations. This will be achieved by generalizing the concept of optimal threshold factors associated with absolutely monotonic functions. Second, to design efficient algebraic algorithms for constructing the optimal threshold polynomials that characterize these methods, avoiding the reliance on complex non-linear optimization. Third, to apply the resulting methods to semi-discretized partial differential equations, demonstrating their practical performance and effectiveness in

preserving qualitative properties in stiff and structure-sensitive problems.

CHAPTER 2

GENERALIZED OPTIMAL THRESHOLD FACTORS, THEORY AND COMPUTATION

The concept of optimal threshold factors was introduced in [33] for the linear space of polynomials that coincide with the Taylor expansion of the exponential function up to a prescribed order, that is, the space of polynomials for which the successive derivatives at the origin are equal to 1. In this chapter, we extend this concept by considering the space of polynomials whose Taylor expansion matches that of a given function (not necessarily the exponential) up to a prescribed order. To maintain consistency in terminology, we continue to refer to these as optimal threshold factors.

This chapter is organized as follows. Section 1 reviews the concepts of absolutely monotonic functions and threshold factors. In Section 2, we introduce the notion of optimal threshold factors and establish an initial bound for them. Section 3 is devoted to proving the existence and uniqueness of the optimal threshold polynomial. In Section 4, we present explicit expressions for low-order optimal threshold polynomials along with their associated factors. Finally, Section 5 outlines an algorithm for their computation based on the concept of blossoming.

2.1 Absolute Monotonicity and Threshold Factors

This section reviews the notion of absolutely monotonic function and threshold factors.

Definition 2.1. *Let $f : [a, b] \rightarrow [0, \infty)$ be a function in $C([a, b]) \cap C^\infty((a, b))$. The function f is said to be absolutely monotonic on $[a, b]$ if*

$$f^{(k)}(x) \geq 0 \quad \text{for all } k \geq 0 \text{ and } x \in [a, b].$$

Let $\Lambda_{p+1} = (\lambda_0, \lambda_1, \dots, \lambda_p)$ be a sequence of positive real numbers. Denote by $\Pi_m(\Lambda_{p+1})$, with $m \geq p$, the set of polynomials ϕ of degree m of the form

$$\phi(x) = \lambda_0 + \frac{\lambda_1}{1!}x + \dots + \frac{\lambda_p}{p!}x^p + a_{p+1}x^{p+1} + \dots + a_mx^m,$$

where $a_{p+1}, a_{p+2}, \dots, a_m$ are arbitrary real numbers. This space can equivalently be described as the set of polynomials ϕ of degree $m \geq p$ such that

$$\phi^{(k)}(0) = \lambda_k \quad \text{for } k = 0, 1, \dots, p.$$

Definition 2.2. *The threshold factor $R(\phi)$ of a polynomial ϕ in $\Pi_m(\Lambda_{p+1})$ is defined as*

$$R(\phi) = \sup\{r \geq 0 \mid \phi \text{ is absolutely monotonic on } [-r, 0]\}.$$

Remark 2.1. *We often use the following fact, if a degree m polynomial ϕ satisfies*

$$\phi^{(k)}(-r) \geq 0 \quad \text{for all } k \geq 0, \tag{2.1}$$

then ϕ is absolutely monotonic on the interval $[-r, 0]$. This follows from the Taylor expansion of ϕ about $x = -r$

$$\phi(x) = \sum_{k=0}^m \frac{\phi^{(k)}(-r)}{k!} (x+r)^k.$$

Hence, if (2.1) holds, then $\phi^{(k)}(x) \geq 0$ for all $x \in [-r, 0]$ and all $k \geq 0$.

We start by establishing the following characterization.

Lemma 2.1. *A polynomial ϕ of degree $m \geq p$ written as*

$$\phi(x) = \sum_{k=0}^m \beta_k \left(1 + \frac{x}{r}\right)^k, \quad \text{with } r > 0, \quad (2.2)$$

belongs to $\Pi_m(\Lambda_{p+1})$ and absolutely monotonic over $[-r, 0]$ if and only if the coefficients $\beta_k, k = 0, 1, \dots, m$, are non-negative and

$$\sum_{k=0}^m (k)_j \beta_k = r^j \lambda_j \quad \text{for } j = 0, 1, \dots, p, \quad (2.3)$$

where

$$(a)_0 := 1 \quad \text{and} \quad (a)_j := a(a-1) \dots (a-j+1) \quad (2.4)$$

is the falling factorial.

Proof. Let ϕ be a polynomial of the form (2.2). We have

$$\phi^{(k)}(-r) = \frac{\beta_k}{r^k} \quad \text{for } k = 0, 1, \dots, m,$$

and

$$\phi^{(j)}(0) = \frac{\sum_{k=0}^m \binom{k}{j} \beta_k}{r^j} \quad \text{for } j = 0, 1, \dots, p.$$

Thus, by remark 2.1, the polynomial ϕ is absolutely monotonic over $[-r, 0]$ and belongs to $\Pi_m(\Lambda_p)$ if and only if the coefficients β_k , $k = 0, 1, \dots, m$, are non-negative and (2.3) holds. $\square$

2.2 Optimal Threshold Factors

This section introduces the concept of optimal threshold factors for finite sequences of positive real numbers and establishes upper and lower bounds for these factors.

Definition 2.3. *The optimal threshold factor $R_m(\Lambda_{p+1})$ is defined by*

$$R_m(\Lambda_{p+1}) = \sup\{R(\phi) \mid \phi \in \Pi_m(\Lambda_{p+1})\}. \quad (2.5)$$

Remark 2.2. *Denote by $\mathbb{B}$ the $(p+1) \times (m+1)$ matrix*

$$\mathbb{B} = (b_{ij}) = (j)_i, \quad 0 \leq i \leq p, \quad 0 \leq j \leq m.$$

Equation (2.3) can be expressed as

$$\mathbb{B}\beta = (\lambda_0, \lambda_1 r, \dots, \lambda_p r^p)^T,$$

where $\beta = (\beta_1, \beta_2, \dots, \beta_m)^T \geq 0$ (here and everywhere else inequalities should be interpreted componentwise). It is shown in [33] that any p columns of the matrix $\mathbb{B}$

are linearly independent.

We now establish a preliminary bound on the optimal threshold factor. The proof of the following proposition is inspired by Theorem 1 in [33].

Proposition 2.1. *Let $\Lambda_{p+1} = (\lambda_0, \lambda_1, \dots, \lambda_p)$ be a sequence of positive real numbers.*

Then, for any integers $m \geq p \geq 1$, the optimal threshold factor satisfies

$$0 < R_m(\Lambda_{p+1}) \leq (m - p + 1) \cdot \frac{\lambda_{p-1}}{\lambda_p}.$$

Proof. Let H_p be the polynomial defined by

$$H_p(x) = \sum_{k=0}^p \frac{\lambda_k}{k!} x^k.$$

This polynomial belongs to $\Pi_m(\Lambda_{p+1})$ and satisfies

$$H^{(j)}(0) = \lambda_j > 0, \quad \text{for } j = 0, 1, \dots, p.$$

By continuity, it follows that $R(H_p) > 0$, and hence $R_m(\Lambda_{p+1}) > 0$.

To prove the upper bound, let $\phi \in \Pi_m(\Lambda_{p+1})$ be absolutely monotonic on $[-r, 0]$ for some $r > 0$. According to Lemma 2.1, ϕ can be written as

$$\phi(x) = \sum_{k=0}^m \beta_k \left(1 + \frac{x}{r}\right)^k,$$

with $\beta_k \geq 0$ for all $k = 0, 1, \dots, m$.

Moreover, we have the relations

$$\phi^{(p-1)}(0) = \sum_{k=0}^m (k)_{p-1} \beta_k = r^{p-1} \lambda_{p-1}, \quad (2.6)$$

$$\phi^{(p)}(0) = \sum_{k=0}^m (k)_p \beta_k = r^p \lambda_p. \quad (2.7)$$

Subtracting $(m - p + 1)$ times Equation (2.6) from Equation (2.7), we obtain

$$0 \geq \sum_{k=0}^m (k)_{p-1} (k - m) \beta_k = r^{p-1} (\lambda_p r - (m - p + 1) \lambda_{p-1}).$$

Therefore,

$$r \leq (m - p + 1) \cdot \frac{\lambda_{p-1}}{\lambda_p},$$

which establishes the desired upper bound. $\square$

2.3 Existence and Uniqueness of Optimal Threshold Polynomials

In this section, we provide a proof of both the existence and uniqueness of the optimal threshold polynomial corresponding to an arbitrary sequence of positive real numbers.

From now on, we denote by Π_p the linear space of real polynomials of degree at most p . The Stirling numbers, $s(n, k)$, of the first kind, and the Stirling numbers,

$S(n, k)$, of the second kind are defined as the coefficients in the expansions

$$(x)_n = \sum_{k=0}^n s(n, k)x^k; \quad x^n = \sum_{k=0}^n S(n, k)(x)_k, \quad n \geq 0; \text{ for any } x \in \mathbb{R}. \quad (2.8)$$

For a given sequence $\Lambda_{p+1} = (\lambda_0, \lambda_1, \dots, \lambda_p)$ of positive real numbers, we define the polynomials

$$B_n(\Lambda_{p+1}, x) = \sum_{k=0}^n S(n, k)\lambda_k x^k.$$

Lemma 2.2. *For any $1 \leq n \leq p$, we have*

$$\sum_{k=0}^n s(n, k)B_k(\Lambda_{p+1}, x) = \lambda_n x^n.$$

Proof. From (2.8), it is clear that for $j = 0, 1, \dots, n$,

$$\sum_{k=0}^n s(n, k)S(k, j) = \delta_{nj}.$$

Thus, we obtain

$$\begin{aligned} \sum_{k=0}^n s(n, k)B_k(\Lambda_{p+1}, x) &= \sum_{k=0}^n \sum_{j=0}^k s(n, k)S(k, j)\lambda_j x^j \\ &= \sum_{j=0}^n \lambda_j x^j \sum_{k=0}^n s(n, k)S(k, j) = \lambda_n x^n. \end{aligned}$$

This concludes the proof. □

For every positive real number R , we define the linear functional

$$\mathcal{L}_R : \Pi_p \longrightarrow \mathbb{R}$$

by setting

$$\mathcal{L}_R [(t)_j] = \lambda_j R^j \quad \text{for } j = 0, 1, \dots, p. \quad (2.9)$$

Using the fact that

$$t^\ell = \sum_{j=0}^{\ell} S(\ell, j) (t)_j,$$

we obtain the moments of the linear form $\mathcal{L}_R$ as

$$\mathcal{L}_R(t^\ell) = B_\ell(\Lambda_{p+1}, R) = \sum_{j=0}^{\ell} S(\ell, j) \lambda_j R^j, \quad \ell = 0, 1, \dots, p.$$

Define the degree p polynomial $\mathcal{H}_p(\cdot; R)$ in x by

$$\mathcal{H}_p(x; R) = \mathcal{L}_R [(x - t)^p]. \quad (2.10)$$

Lemma 2.3. *The polynomial $\mathcal{H}_p(\cdot; R)$ is given by*

$$\mathcal{H}_p(x; R) = \sum_{k=0}^p (-1)^{p-k} \binom{p}{k} B_{p-k}(\Lambda_{p+1}, R) x^k, \quad (2.11)$$

where

$$B_\ell(\Lambda_{p+1}, R) = \sum_{j=0}^{\ell} S(\ell, j) \lambda_j R^j. \quad (2.12)$$

Proof. Using the fact that $\mathcal{L}_R[t^\ell] = B_\ell(R)$, we obtain

$$\mathcal{L}_R[(x-t)^p] = \sum_{k=0}^p (-1)^{p-k} \binom{p}{k} x^k \mathcal{L}_R(t^{p-k}) = \sum_{k=0}^p (-1)^{p-k} \binom{p}{k} B_{p-k}(R) x^k.$$

This concludes the proof. □

Theorem 2.1. *Given a sequence $\Lambda_{p+1} = (\lambda_0, \lambda_1, \dots, \lambda_p)$ of positive real numbers and for any $m \geq p$, the optimal threshold factor $R_m(\Lambda_{p+1})$ is the supremum of positive real numbers R for which the polynomial $\mathcal{H}_p(\cdot; R)$ admits a representation of the form*

$$\mathcal{H}_p(x; R) = \sum_{i=1}^s \alpha_i (x - m_i)^p, \quad s \geq 1, \quad (2.13)$$

with integers $0 \leq m_1 < m_2 < \dots < m_s \leq m$ and non-negative real numbers $\alpha_1, \alpha_2, \dots, \alpha_s$.

Proof. Let $R > 0$ be such that the polynomial $\mathcal{H}_p(\cdot; R)$ admits a representation of the form

$$\mathcal{H}_p(x; R) = \sum_{i=1}^s \alpha_i (x - m_i)^p, \quad s \geq 1, \quad (2.14)$$

with integers $0 \leq m_1 < m_2 < \dots < m_s \leq m$ and non-negative real numbers $\alpha_1, \alpha_2, \dots, \alpha_s$. From the polynomial expression of $\mathcal{H}_p(x; R)$, it follows that

$$\sum_{k=1}^s \alpha_k m_k^\ell = B_\ell(\Lambda_{p+1}, R), \quad \ell = 0, 1, \dots, p.$$

Denote by ϕ the polynomial

$$\phi(x) = \sum_{k=1}^s \alpha_k \left(1 + \frac{x}{R}\right)^{m_k}.$$

It is clear that $\phi^{(j)}(-R) \geq 0$ for any $j \geq 0$, and from Lemma 2.2,

$$\phi^{(\ell)}(0) = \frac{1}{R^\ell} \sum_{k=1}^s \alpha_k (m_k)_\ell = \frac{1}{R^\ell} \sum_{j=0}^{\ell} s(\ell, j) \sum_{k=1}^s \alpha_k m_k^j = \frac{1}{R^\ell} \sum_{j=0}^{\ell} s(\ell, j) B_j(\Lambda_{p+1}, R) = \lambda_\ell.$$

Thus, ϕ belongs to $\Pi_m(\Lambda_{p+1})$ and is absolutely monotonic over $[-R, 0]$ and therefore, $R \leq R_m(\Lambda_{p+1})$. Moreover, if a polynomial

$$\sum_{k=1}^s \alpha_k \left(1 + \frac{x}{R_m(\Lambda_{p+1})}\right)^{m_k}$$

with integers $0 \leq m_1 < m_2 < \dots < m_s \leq m$, belongs to $\Pi_m(\Lambda_{p+1})$ and is absolutely monotonic over $[-R_m(\Lambda_p), 0]$, then the polynomial $\sum_{i=1}^s \alpha_i (x - m_i)^p$ satisfies the condition of the theorem and coincides with $\mathcal{H}_p(x; R_m(\Lambda_{p+1}))$. $\square$

Remark 2.3. *The previous theorem can be re-stated as saying that the optimal threshold factor $R_m(\Lambda_{p+1})$ is the supremum of positive real number R such that the linear form $\mathcal{L}_R$ admits a positive quadrature with integer nodes not exceeding m , and exact for all polynomials of degree at most p .*

We now state and prove an existence result.

Theorem 2.2. *There exists a polynomial $\Phi_m(\Lambda_{p+1})$ in $\Pi_m(\Lambda_{p+1})$ such that*

$$R(\Phi_m(\Lambda_{p+1})) = R_m(\Lambda_{p+1}).$$

Proof. Denote by C the closed cone generated by the columns of the matrix $\mathbb{B}$ of

Remark 2.2. Thus, the optimal threshold factor $R_m(\Lambda_{p+1})$ is given by

$$R_m(\Lambda_{p+1}) = \sup\{r \mid r = 0 \text{ or } r > 0, (\lambda_0, \lambda_1 r, \dots, \lambda_p r^p) \in C\}. \quad (2.15)$$

Since, by Proposition 2.1, $0 < R_m(\Lambda_{p+1}) < \infty$, the supremum in (2.15) is taken over a compact subset of C .

□

To prove the uniqueness of the optimal threshold polynomial, we shall first show that the number of summands in the representation (2.13) is at most p .

Theorem 2.3. *For any positive integers m and p such that $m \geq p$, there exist integers $0 \leq m_1 < m_2 < \dots < m_p \leq m$ and non-negative real numbers $\alpha_1, \alpha_2, \dots, \alpha_p$, such that*

$$\mathcal{H}_p(x; R_m(\Lambda_{p+1})) = \sum_{i=1}^p \alpha_i (x - m_i)^p. \quad (2.16)$$

Proof. Let us assume that $\mathcal{H}_p(x; R_m(\Lambda_{p+1})) = \sum_{i=1}^s \alpha_i (x - m_i)^p$ with $s > p$ and $\alpha_i > 0, i = 1, 2, \dots, s$. Write

$$\sum_{i=1}^p \alpha_i (x - m_i)^p = \mathcal{H}_p(x; R_m(\Lambda_{p+1})) - \sum_{i=p+1}^s \alpha_i (x - m_i)^p. \quad (2.17)$$

Equation (2.17) can be viewed as a linear system in $(\alpha_1, \alpha_2, \dots, \alpha_p)$, i.e.,

$$\sum_{i=1}^p \alpha_i m_i^j = B_j(\Lambda_{p+1}, R_m(\Lambda_{p+1})) - \sum_{i=p+1}^s \alpha_i m_i^j, \quad j = 0, 1, \dots, p,$$

that has a positive solution, $\alpha_i > 0$, $i = 1, 2, \dots, p$. Therefore, there exists an $\epsilon > 0$ such that the linear system in $(\beta_1, \beta_2, \dots, \beta_p)$

$$\sum_{i=1}^p \beta_i (x - m_i)^p = \mathcal{H}_p(x; R_m(\Lambda_{p+1}) + \epsilon) - \sum_{i=p+1}^s \alpha_i (x - m_i)^p$$

also has a positive solution. Thus, we obtain

$$\mathcal{H}_p(x; R_m(\Lambda_{p+1}) + \epsilon) = \sum_{i=1}^p \beta_i (x - m_i)^p + \sum_{i=p+1}^s \alpha_i (x - m_i)^p.$$

This contradicts the definition of $R_m(\Lambda_{p+1})$ as given in Theorem 2.1.

□

We are now in a position to prove the uniqueness of the optimal threshold polynomial.

Corollary 2.1. *There exists a unique polynomial $\Phi_m(\Lambda_{p+1})$ in $\Pi_m(\Lambda_{p+1})$ such that*

$$R(\Phi_m(\Lambda_{p+1})) := R_m(\Lambda_{p+1}).$$

Proof. For $x \in \mathbb{R}^m$, we shall denote by $\|x\|_0 := \text{Card}(\text{supp}(x))$. Let us assume that there exist two different polynomials ϕ_1 and ϕ_2 such that $R(\phi_1) = R(\phi_2) = R_m(\Lambda_{p+1})$.

Thus, there exists non-negative vectors α, β in $\mathbb{R}^m$ such that

$$\mathbb{B}\alpha = \mathbb{B}\beta = (\lambda_0, \lambda_1 R_m(\Lambda_{p+1}), \dots, \lambda_p R_m^p(\Lambda_{p+1}))$$

and such that $\|\alpha\|_0 \leq p$ and $\|\beta\|_0 \leq p$. As $\mathbb{B}((\alpha + \beta)/2) = R_m(\Lambda_{p+1})$, we have $\|\alpha - \beta\|_0 \leq p$ and $\mathbb{B}(\alpha - \beta) = 0$. Since every $p + 1$ columns of $\mathbb{B}$ are linearly independent, we conclude that $\alpha = \beta$. This contradiction proves the uniqueness of the optimal threshold polynomial.

□

2.4 Optimal Threshold Polynomials of Low Orders

Building upon the upper bound provided by Proposition 2.1, this section presents the optimal threshold factors and their associated polynomials for sequences of length two and three.

Proposition 2.2. *For any sequence $\Lambda_2 = (\lambda_0, \lambda_1)$ of positive real numbers and any integer $m \geq 1$, we have*

$$R_m(\Lambda_2) = m \frac{\lambda_0}{\lambda_1} \quad \text{and} \quad \Phi_m(\Lambda_2)(x) = \lambda_0 \left(1 + \frac{\lambda_1 x}{m \lambda_0} \right)^m.$$

Proof. The polynomial $\Phi_m(\Lambda_2)$ belongs to $\Pi_m(\Lambda_2)$ and is clearly absolutely monotonic over the interval $[-m\lambda_0/\lambda_1, 0]$. Thus, $R_m(\Lambda_2) \geq m\lambda_0/\lambda_1$. Moreover, Proposition 2.1 states that $R_m(\Lambda_2) \leq m\lambda_0/\lambda_1$. Hence, the result. □

Proposition 2.3. *For any sequence $\Lambda_3 = (\lambda_0, \lambda_1, \lambda_2)$ of positive real numbers and any integer $m \geq 2$ such that*

$$\lambda_0 \geq \frac{\lambda_1^2(m-1)}{\lambda_2 m}, \quad (2.18)$$

we have

$$R_m(\Lambda_3) = (m-1) \frac{\lambda_1}{\lambda_2},$$

and

$$\Phi_m(\Lambda_3)(x) = \left(\lambda_0 - \frac{\lambda_1^2(m-1)}{m\lambda_2} \right) + \frac{\lambda_1^2(m-1)}{m\lambda_2} \left(1 + \frac{\lambda_2 x}{(m-1)\lambda_1} \right)^m.$$

Proof. The polynomial $\Phi_m(\Lambda_3)$ belongs to $\Pi_m(\Lambda_3)$ and is absolutely monotonic over the interval $[-(m-1)\lambda_1/\lambda_2, 0]$ when condition 2.18 holds. Thus, $R_m(\Lambda_3) \geq (m-1)\lambda_1/\lambda_2$. Moreover, Proposition 2.1 states that $R_m(\Lambda_3) \leq (m-1)\lambda_1/\lambda_2$. This concludes the proof. $\square$

Remark 2.4. *When condition (2.18) does not hold, the optimal threshold factor is different from the one stated in the previous proposition. For instance, using the algorithm in the next section, we find that for the sequence $\Lambda_3 = (1, 2, 3)$ and $m = 4$, we have*

$$R_4(\Lambda_3) = 2 \quad \text{and} \quad \Phi_4(\Lambda_3)(x) = \left(1 + \frac{x}{2} \right)^4.$$

2.5 Polar Forms and an Algorithm for Computing Optimal Threshold Factors

Polar forms [38] are valuable tools in many mathematical disciplines [43], [44]. This section provides a concise review of their definition and subsequently demonstrates their application in developing an algorithm for computing optimal threshold factors. The presented algorithm can be viewed as a generalization of Kraijenvanger's algorithm in [33].

Definition 2.4. *Given a real polynomial P of degree at most n , there exists a unique symmetric multi-affine function $p(u_1, u_2, \dots, u_n)$ such that $p(x^{[n]}) = P(x)$ for any $x \in \mathbb{R}$. The function p is called the blossom or the polar form of the polynomial P .*

The polar form of a polynomial P expressed in the monomial basis as $P(x) = \sum_{k=0}^n a_k x^k$ is given by

$$p(u_1, u_2, \dots, u_n) = \sum_{k=0}^n a_k \sigma_k(u_1, u_2, \dots, u_n),$$

where σ_k denotes the normalized k -th elementary symmetric polynomial

$$\sigma_k(u_1, u_2, \dots, u_n) = \binom{n}{k}^{-1} \sum_{1 \leq j_1 < \dots < j_k \leq n} u_{j_1} u_{j_2} \dots u_{j_k}.$$

When the polynomial P is of the form

$$P(x) = \sum_{k=1}^s \alpha_k (x - a_k)^n,$$

then its polar form is given by

$$p(u_1, u_2, \dots, u_n) = \sum_{k=1}^s \alpha_k \prod_{i=1}^n (u_i - a_k). \quad (2.19)$$

We are now in a position to describe the algorithm for computing the optimal threshold factor $R_m(\Lambda_{p+1})$ and the associated polynomial $\Phi_m(\Lambda_{p+1})$, for any sequence of positive real numbers $\Lambda_{p+1} = (\lambda_0, \lambda_1, \dots, \lambda_p)$ and any integer $m \geq p$. The main idea of the algorithm is that the number of summands in the representation (2.16) is at most p .

If we write the polynomial $\mathcal{H}_p(., R)$ in the form

$$\mathcal{H}_p(x; R) = \sum_{i=1}^p \alpha_i (x - m_i)^p, \quad (2.20)$$

and denote by $h_p(u_1, u_2, \dots, u_p; R)$ the value at $(u_1, u_2, \dots, u_n)$ of the polar form of $\mathcal{H}_p(., R)$ (as in (2.19)), we obtain

$$h_n(m_1, m_2, \dots, m_n; R) = 0. \quad (2.21)$$

This shows that for any choice of non-negative integers $m_1, m_2, \dots, m_p$ less than m , Equation (2.21) provides a polynomial in R of degree p whose positive real roots are candidates for the optimal threshold factor $R_m(\Lambda_{p+1})$. For each such R , we must verify the non-negativity of the coefficients $\alpha_1, \alpha_2, \dots, \alpha_p$ in the representation (2.20).

A simple expression for these coefficients can be obtained by evaluating the polar

form of both sides of (2.20) at $(m_1, m_2, \dots, m_{k-1}, m+1, m_{k+1}, \dots, m_n)$, yielding

$$\alpha_k = \frac{h_n(m_1, m_2, \dots, m_{k-1}, m+1, m_{k+1}, \dots, m_n; R)}{(m+1-m_k) \prod_{i=1, i \neq k}^n (m_i - m_k)}, \quad k = 1, 2, \dots, n. \quad (2.22)$$

Based on (2.21) and (2.22), an algorithm for computing $R_m(\Lambda_{p+1})$ and the associated optimal threshold polynomial proceeds as follows.

- **Step 1** Generate all strictly increasing integer sequences M of length p , with $0 \leq m_1 < m_2 < \dots < m_p \leq m$. For each sequence M , find all positive solutions R to the polynomial equation (2.21).
- **Step 2** For each real number R obtained in Step 1, verify the non-negativity of the coefficients α_k using (2.22). Retain only those pairs (R, M) for which all coefficients α_k are non-negative.
- **Step 3** $R_m(\Lambda_{p+1})$ is the largest value of R remaining after Step 2. The corresponding optimal threshold polynomial is given by

$$\Phi_m(\Lambda_{p+1})(x) = \sum_{k=1}^p \alpha_k \left(1 + \frac{x}{R_m(\Lambda_{p+1})} \right)^{m_k},$$

where $(m_1, m_2, \dots, m_p)$ is the integer sequence associated with $R_m(\Lambda_{p+1})$, and α_k are the coefficients computed in Step 2.

The computational cost of the above algorithm increases exponentially as the values of m and p grow. Therefore, its practical use is limited to cases where m and p are relatively small. In a forthcoming contribution, we will explore more efficient algo-

rithms for computing these threshold factors using the theory of Christoffel transforms of orthogonal polynomials.

Example 2.1. *The table below provides the values of the optimal threshold factors for various sequences Λ_3 as computed using our algorithm.*

Λ_4	$R_4(\Lambda_4)$	$R_5(\Lambda_4)$	$R_6(\Lambda_4)$	$R_7(\Lambda_4)$	$R_8(\Lambda_4)$
(1, 1, 1, 1)	2	2.6506	3.5184	4.2879	5.1071
(2, 2, 1, 1)	1.2778	1.3210	1.3556	1.3844	1.4088
(1, 2, 3, 4)	1	1.25	1.3177	1.3930	1.5
(2, 1, 1, 1)	2	3	4	5	6
(2, 2, 2, 1)	2	2	2	2	2

Table 2.1: Values of the optimal threshold factors for various sequences Λ_3 as computed by our algorithm.

A few remarks concerning the table are in order

1. The proposed algorithm also provides the corresponding optimal threshold polynomials. For instance, for the sequence $\Lambda_4 = (1, 2, 3, 4)$, we have $R_5(\Lambda_4) = 1.25$, and the associated polynomial is given by

$$\Phi_5(\Lambda_3)(x) = \alpha_1 \left(1 + \frac{x}{1.25}\right)^2 + \alpha_2 \left(1 + \frac{x}{1.25}\right)^3 + \alpha_3 \left(1 + \frac{x}{1.25}\right)^5,$$

with

$$(\alpha_1, \alpha_2, \alpha_3) = (0.72917, 0.15625, 0.11458).$$

For the sequence $\Lambda_4 = (2, 2, 1, 1)$, we have $R_7(\Lambda_4) = 1.3844$, and

$$\Phi_7(\Lambda_3)(x) = \alpha_1 \left(1 + \frac{x}{1.3844}\right) + \alpha_2 \left(1 + \frac{x}{1.3844}\right)^2 + \alpha_3 \left(1 + \frac{x}{1.3844}\right)^7,$$

with

$$(\alpha_1, \alpha_2, \alpha_3) = (1.2944, 0.69292, 0.012634).$$

2. The table also reveals that for the sequence $\Lambda_4 = (2, 2, 2, 1)$, we have

$$R_m(\Lambda_4) = 2 \quad \text{for } m = 4, 5, 6, 7, 8.$$

In fact, for this sequence, we have $R_m(\Lambda_4) = 2$ for all $m \geq 3$, and

$$\Phi_m(\Lambda_4)(x) = \frac{2}{3} + \frac{4}{3} \left(1 + \frac{x}{2}\right)^3. \quad (2.23)$$

Moreover, the polynomial in (2.23) is the unique absolutely monotonic function on the interval $[-2, 0]$ with the prescribed derivatives at the origin. This result can be proven using the theory of Bernstein as detailed in [32].

3. The table also reveals that for the sequence $\Lambda_4 = (2, 1, 1, 1)$, we have

$$R_m(\Lambda_4) = m - 2 \quad \text{for } m = 4, 5, 6, 7, 8.$$

This observation can be generalized in the following theorem.

Theorem 2.4. *Let $m \geq 3$ be an integer, and let $\Lambda_4 = (a, b, b, b)$, where a and b are positive real numbers such that*

$$m(m-1)a \geq 2b(m-2). \quad (2.24)$$

Then,

$$R_m(\Lambda_4) = m - 2,$$

and

$$\Phi_m(\Lambda_4)(x) = \alpha_1 + \alpha_2 \left(1 + \frac{x}{m-2}\right) + \alpha_3 \left(1 + \frac{x}{m-2}\right)^m, \quad (2.25)$$

where

$$\alpha_1 = a - \frac{2(m-2)b}{m}, \quad \alpha_2 = \frac{(m-2)b}{m-1}, \quad \text{and} \quad \alpha_3 = \frac{(m-2)^2b}{m(m-1)}.$$

Proof. According to Proposition 2.1, $R_m(\Lambda_4) \leq m - 2$. Moreover, under condition (2.24), the polynomial in (2.25) is absolutely monotonic on the interval $[-(m-2), 0]$ and satisfies the prescribed derivatives at the origin. $\square$

Another interesting conclusion that can be drawn from the previously described algorithm for computing the optimal threshold factor is as follows.

Theorem 2.5. *If the elements of the sequence Λ_{p+1} are positive rational integers, then for any integer m such that $m \geq p$, the optimal threshold factor $R_m(\Lambda_{p+1})$ is an algebraic number.*

Proof. From (2.12), if the elements of the sequence Λ_{p+1} are positive rational integers, then the polynomial in R given in (2.11) has rational coefficients. Since the optimal threshold factor is the largest positive root of a polynomial of the form

$$h_n(m_1, m_2, \dots, m_p; R),$$

where $m_1, m_2, \dots, m_p$ are non-negative integers, we conclude that the optimal thresh-

old factor is an algebraic number.

□

CHAPTER 3

A NEW FAMILY OF DISCRETE ORTHOGONAL POLYNOMIALS

It has been established in Theorem 2.2 that there exists a polynomial $\Phi_m(\Lambda_{p+1}) \in \Pi_m(\Lambda_{p+1})$ such that

$$R_m(\Lambda_{p+1}) = R(\Phi_m(\Lambda_{p+1})). \quad (3.1)$$

Furthermore, Lemma 2.1 shows that a polynomial of the form (2.2) belongs to $\Pi_m(\Lambda_{p+1})$ and is absolutely monotonic over $[-R, 0]$ if and only if its coefficients β_k are nonnegative and satisfy the "discrete moment type" equations

$$\sum_{k=0}^m \beta_k k^j = \sum_{\ell=0}^j S(j, \ell) \lambda_\ell R^\ell, \quad j = 0, 1, \dots, p, \quad (3.2)$$

where $S(j, \ell)$ are the Stirling numbers of the second kind. A key observation is that the left-hand side of (3.2) represents a quadrature formula with integer nodes. This suggests that one should seek a measure for which the right-hand side corresponds to its moments. Building upon this structural insight, we introduce a *novel discrete*

measure, enabling us to rewrite Equation (3.2) as a moment equation. This representation provides deeper insights into the optimal threshold factors and facilitates the derivation of sharp bounds for them.

This chapter is organized as follows. Section 3.1 introduces a new discrete measure and explores its structural properties. We demonstrate that the generalized Poisson-Charlier, Meixner, and Krawtchouk measures arise as special cases of this measure. In Section 3.2, we derive the three-term recurrence relations for the associated discrete orthogonal polynomials and establish sufficient conditions for the monotonicity of their zeros. Section 3.3 elucidates the connection between the newly introduced discrete orthogonal polynomials and optimal threshold factors.

3.1 A New Discrete Measure Associated with Absolutely Monotonic Functions

Definition 3.1. *Given R_∞ in $\bar{\mathbb{R}} := \mathbb{R} \cup \{\infty\}$ and an absolutely monotonic function F over the interval $[-R_\infty, 0]$, we define the discrete measure μ_R^F , supported on the set of nonnegative integers, as*

$$\mu_R^F = \sum_{j=0}^{\infty} \frac{F^{(j)}(-R) R^j}{j!} \delta_j, \quad 0 \leq R \leq R_\infty, \quad (3.3)$$

where δ_j denotes the Dirac measure centered at j .

Since the function F is absolutely monotonic over the interval $[-R_\infty, 0]$, the measure μ_R^F is positive for any R such that $0 \leq R \leq R_\infty$. By definition, the integral of a

given function f with respect to the discrete measure μ_R^F is given by

$$\int f(t) d\mu_R^F(t) = \sum_{j=0}^{\infty} \frac{F^{(j)}(-R) R^j}{j!} f(j) \quad (3.4)$$

provided that the infinite sum converges.

Remark 3.1. *Since the function F is absolutely monotonic over the interval $[-R_{\infty}, 0]$, all its derivatives are also absolutely monotonic over the same interval. Consequently, for any positive integer ℓ , the measure*

$$\mu_R^{F^{(\ell)}} = \sum_{j=0}^{\infty} \frac{F^{(j+\ell)}(-R) R^j}{j!} \delta_j, \quad (3.5)$$

is positive for any R such that $0 \leq R \leq R_{\infty}$.

The following lemma shows that moments of the measure μ_R^F of all orders are finite.

Proposition 3.1. *The moments $m_k^F(R), k \geq 0$, of the measure μ_R^F are given by*

$$m_k^F(R) := \int t^k d\mu_R^F = \sum_{j=0}^k S(k, j) R^j F^{(j)}(0), \quad (3.6)$$

where $S(., .)$ are the Stirling numbers of the second kind.

Proof. By Taylor expansion, we have

$$\int (t)_j d\mu_R^F = \sum_{k=0}^{\infty} \frac{F^{(k)}(-R) R^k (k)_j}{k!} = R^j \sum_{k=0}^{\infty} \frac{F^{(j+k)}(-R) R^k}{k!} = R^j F^{(j)}(0).$$

We conclude the proof using the formula $t^{\ell} = \sum_{j=0}^{\ell} S(\ell, j)(t)_j$. □

We shall need the following proposition.

Proposition 3.2. *For $k = 0, 1, 2, \dots, p$, the following relation holds*

$$\int (t)_k g(t) d\mu_R^F = R^k \int g(t+k) d\mu_R^{F^{(k)}}. \quad (3.7)$$

where $(t)_k$ denotes the falling factorial.

Proof. Using the definition of μ_R^F and the identity $(j)_k = \frac{j!}{(j-k)!}$, we obtain

$$\int (t)_k g(t) d\mu_R^F = \sum_{j=k}^{\infty} \frac{F^{(j)}(-R)R^j}{(j-k)!} g(j),$$

Therefore,

$$\int (t)_k g(t) d\mu_R^F = R^k \sum_{t=0}^{\infty} \frac{F^{(t+k)}(-R)R^t}{t!} g(t+k) = R^k \int g(t+k) d\mu_R^{F^{(k)}}.$$

This concludes the proof. □

Several known discrete measures coincide with the measure μ_R^F , as demonstrated in the following.

Example 3.1. Poisson-Charlier Measures. *The function $F(x) = e^x$ is absolutely monotonic over the interval $(-\infty, 0]$ and the associated measure μ_R^F is given by the Poisson-Charlier measure*

$$\mu_R^F = \sum_{k=0}^{\infty} \frac{e^{-R}R^k}{k!} \delta_k, \quad R \in [0, \infty).$$

Example 3.2. Generalised Poisson-Charlier Measures. *The function*

$$F(x) = e^{\alpha x}$$

is absolutely monotonic over the interval $(-\infty, 0]$ and the associated measure μ_R^F is given by the generalized Poisson-Charlier measure

$$\mu_R^F = \sum_{k=0}^{\infty} \frac{e^{-\alpha R} \alpha^k R^k}{k!} \delta_k, \quad R \in [0, \infty). \quad (3.8)$$

Example 3.3. Meixner Measures. *The function*

$$F(x) = (1 - x)^{-\beta}$$

is absolutely monotonic over the interval $(-\infty, 0]$. Moreover, we have

$$F^{(k)}(-R) = \frac{(\beta)_k}{(1 + R)^{\beta+k}}.$$

Therefore, the associated measure μ_R^F is given by the Meixner measure

$$\mu_R^F = \frac{1}{(1 + R)^\beta} \sum_{k=0}^{\infty} \frac{(\beta)_k c^k}{k!} \delta_k, \quad R \in [0, \infty), \quad c = \frac{R}{1 + R}. \quad (3.9)$$

Example 3.4. Krawtchouk Measures. *The function $F(x) = (1 + x)^N$, $N \in \mathbb{N}$,*

is absolutely monotonic in the interval $[-1, 0]$. Moreover, we have

$$F^{(k)}(-R) = \frac{N!}{(N-k)!} (1+R)^{N-k}.$$

The associated measure μ_R^F is given by the Krawtchouk measure

$$\mu_R^F = (1+R)^N \sum_{k=0}^N \binom{N}{k} p^k \delta_k, \quad 0 < p = \frac{R}{1+R} < 1. \quad (3.10)$$

Since the measure μ_R^F is positive with finite moment of all orders, it gives rise to an associated family of discrete orthogonal polynomials $\pi_k^F(\cdot; R)$, $k = 0, 1, \dots$, which satisfies the orthogonality conditions

$$\int \pi_i^F(t; R) \pi_j^F(t; R) d\mu_R(t) = 0 \quad \text{if } i \neq j.$$

Equivalently, these conditions can be expressed as

$$\sum_{k=0}^{\infty} \frac{F^{(k)}(-R) R^k}{k!} \pi_i^F(k; R) \pi_j^F(k; R) = 0 \quad \text{if } i \neq j.$$

An explicit expression of the orthogonal polynomial $\pi_k^F(t; R)$ is given in terms of the

moments of the measure μ_R^F as

$$\pi_k^F(t; R) = C_k \det \begin{pmatrix} m_0^F & m_1^F & \cdots & m_k^F \\ m_1^F & m_2^F & \cdots & m_{k+1}^F \\ \vdots & \vdots & \ddots & \vdots \\ m_{k-1}^F & m_k^F & \cdots & m_{2k-1}^F \\ 1 & t & \cdots & t^k \end{pmatrix}, \quad (3.11)$$

where C_k are arbitrary real constants. From now on, we shall choose the constants C_k such that the orthogonal polynomials $\pi_k^F(t; R)$ are monic polynomials.

3.2 Three-Term Recurrence Relations

We shall need algorithms to compute the zeros of the orthogonal polynomials $\pi_i^F(t; R)$. Directly using the expression (3.11) for this computation is neither numerically stable nor computationally efficient. Instead, reliable algorithms such as the Golub-Welsch method depend on determining the three-term recurrence coefficients associated with these orthogonal polynomials. The derivation of these coefficients is the main goal of this section. More precisely, we shall express the recurrence coefficients of the orthogonal polynomials associated with the measure μ_R^F in terms of the ones associated with $\mu_R^{F'}$.

The monic orthogonal polynomials π_p^F associated with the measure μ_R^F satisfy the

three-terms recurrence

$$t\pi_p^F(t; R) = \pi_{p+1}^F(t; R) + b_p^F \pi_p^F(t; R) + c_p^F \pi_{p-1}^F(t; R), \quad (3.12)$$

where

$$b_p^F = (\gamma_p^F)^2 \int t(\pi_p^F(t; R))^2 d\mu_R^F, \quad c_p^F = (\gamma_{p-1}^F)^2 \int t\pi_p^F(t; R)\pi_{p-1}^F(t; R) d\mu_R^F,$$

and where for any $k \geq 0$, γ_k^F is defined as

$$\gamma_k^F = \frac{1}{\sqrt{\int (\pi_k^F(t; R))^2 d\mu_R^F}}.$$

Writing $\pi_p^F(t+1; R)$ as

$$\pi_p^F(t+1; R) = \sum_{j=0}^p A_{p,j} \pi_j^{F'}(t; R),$$

and using (3.7), we obtain

$$\frac{A_{p,j}}{(\gamma_j^{F'})^2} = \int \pi_p^F(t+1; R) \pi_j^{F'}(t; R) d\mu_R^{F'} = \frac{1}{R} \int \pi_p^F(t; R) t \pi_j^{F'}(t-1; R) d\mu_R^F. \quad (3.13)$$

Thus, by orthogonality, if $j \leq p-1$, $A_{p,j} = 0$. Therefore, we obtain

$$\pi_p^F(t+1; R) = A_{p,p} \pi_p^{F'}(t; R) + A_{p,p-1} \pi_{p-1}^{F'}(t; R). \quad (3.14)$$

Comparing the leading terms in (3.14), we get $A_{p,p} = 1$. Moreover, writing

$$t\pi_{p-1}^{F'}(t-1; R) = \alpha\pi_p^F(t; R) + \sum_{k=1}^p \beta_k \pi_{p-k}^F(t; R), \quad (3.15)$$

and comparing the leading coefficient, we conclude that $\alpha = 1$. Thus integrating (3.15) and using (3.13), we obtain

$$\frac{1}{(\gamma_p^F)^2} = \int \pi_p^F(t; R) t \pi_{p-1}^{F'}(t-1; R) d\mu_R^F = R \frac{A_{p,p-1}}{(\gamma_{p-1}^{F'})^2}.$$

Therefore, we conclude that

$$A_{p,p-1} = \frac{1}{R} B_p^F \quad \text{with} \quad B_p^F = \left(\frac{\gamma_{p-1}^{F'}}{\gamma_p^F} \right)^2.$$

In summary, we have the following.

Theorem 3.1. *The monic orthogonal polynomials $\pi^F(.; R)$ and $\pi^{F'}(.; R)$ satisfy the difference equation*

$$\pi_p^F(t+1; R) = \pi_p^{F'}(t; R) + \frac{1}{R} B_p^F \pi_{p-1}^{F'}(t; R) \quad \text{with} \quad B_p^F = \left(\frac{\gamma_{p-1}^{F'}}{\gamma_p^F} \right)^2. \quad (3.16)$$

Example 3.5. *For the Charlier-Poisson measure associated with the function $F(x) = e^x$ and since $F'(x) = F(x)$, Theorem 3.1 provides the following well-known relation for Charlier-Poisson orthogonal polynomials*

$$\pi_p^F(t+1; R) = \pi_p^F(t; R) + \frac{1}{R} B_p^F \pi_{p-1}^F(t; R).$$

We are now in a position to derive the relation between the three-term recurrence coefficients of the orthogonal polynomials π_k^F and those of $\pi_k^{F'}$.

Theorem 3.2. *The three-term recurrence coefficients associated with π_k^F and those associated with $\pi_k^{F'}$ satisfy*

$$\begin{aligned} (c_{p+1}^F - c_p^{F'})(c_p^F - c_p^{F'}) &= c_p^{F'}(b_p^F - b_p^{F'} - 1)(b_p^F - b_{p-1}^{F'} - 1), \\ (c_{p+1}^{F'} - c_p^F)(c_{p+1}^F - c_{p+1}^{F'}) &= c_{p+1}^F(b_p^F - b_p^{F'} - 1)(b_{p+1}^F - b_p^{F'} - 1). \end{aligned} \quad (3.17)$$

Proof. From the three-term recurrence relation, we have

$$(t+1)\pi_p^F(t+1; R) = \pi_{p+1}^F(t+1; R) + b_p^F \pi_p^F(t+1; R) + c_p^F \pi_{p-1}^F(t+1; R).$$

Thus, from Theorem 3.2, we have

$$\begin{aligned} (t+1)\pi_p^F(t+1; R) &= \pi_{p+1}^{F'}(t; R) + \left(\frac{B_{p+1}^F}{R} + b_p^F \right) \pi_p^{F'}(t; R) + \left(\frac{B_p^F b_p^F}{R} + c_p^F \right) \pi_{p-1}^{F'}(t; R) \\ &\quad + \left(\frac{B_{p-1}^F c_p^F}{R} \right) \pi_{p-2}^{F'}(t; R). \end{aligned} \quad (3.18)$$

Moreover, from Theorem 3.2, we have

$$(t+1)\pi_p^F(t+1; R) = (t+1) \left(\pi_p^{F'}(t; R) + \frac{1}{R} B_p^F \pi_{p-1}^{F'}(t; R) \right).$$

Applying the three-term recurrence relation associated with $\pi_k^{F'}(.; R)$ to the previous

equation yield

$$\begin{aligned}
(t+1)\pi_p^F(t+1; R) &= \pi_{p+1}^{F'}(t; R) + \left(1 + \frac{B_p^F}{R} + b_p^{F'}\right) \pi_n^{F'}(t; R) \\
&+ \left(\frac{B_p^F(1 + b_{p-1}^{F'})}{R} + c_p^{F'}\right) \pi_{p-1}^{F'}(t; R) + \left(\frac{B_p^F c_{p-1}^{F'}}{R}\right) \pi_{p-2}^{F'}(t; R).
\end{aligned} \tag{3.19}$$

Comparing (3.18) and (3.19), we obtain

$$\begin{aligned}
\frac{B_{p+1}^F}{R} + b_p^F &= 1 + \frac{B_p^F}{R} + b_p^{F'}, \\
\frac{B_p^F b_p^F}{R} + c_p^F &= \frac{B_p^F(1 + b_{p-1}^{F'})}{R} + c_p^{F'}, \\
\frac{B_{p-1}^F c_p^F}{R} &= \frac{B_p^F c_{p-1}^{F'}}{R}.
\end{aligned} \tag{3.20}$$

Using the third equality in (3.20) we obtain

$$c_{p+1}^F - c_p^{F'} = \left(\frac{B_{p+1}^F}{B_p^F} - 1\right) c_p^{F'}.$$

Using second equality in (3.20), we get

$$c_p^F - c_p^{F'} = \frac{B_p^F}{R} (1 + b_{p-1}^{F'} - b_p^F).$$

Thus, we obtain

$$(c_{p+1}^F - c_p^{F'})(c_p^F - c_p^{F'}) = c_p^{F'} (1 + b_{p-1}^{F'} - b_p^F) \left(\frac{B_{p+1}^F}{R} - \frac{B_p^F}{R}\right).$$

Thus, using the first equality in (3.20), we obtain the first equality in (3.17). Similar manipulations lead to the second equality in (3.17). $\square$

In what follows, we shall show that if the function F is absolutely monotonic on the interval $(-\infty, 0]$, then the zeros of the orthogonal polynomial $\pi_k^F(\cdot; R)$ increase monotonically with respect to the parameter R . Several preliminary results are necessary to establish the proof.

Theorem 3.3. [45] *Let $\mathcal{N}$ be a subset of the integers. For every $R \in (R_1, R_2)$, let $\{p_n(t, R)\}_{n=0}^\infty$ be a sequence of polynomials orthogonal with respect to a positive weight function with continuous partial derivative $\frac{\partial \omega_R(t; R)}{\partial R}$ for all $R \in (R_1, R_2)$ and $t \in \mathcal{N}$. Suppose further that for each $j = 0, \dots, 2n-1$, the series*

$$\sum_{k \in \mathcal{N}} k^j \omega_R(k; R) \tag{3.21}$$

converges uniformly in R over every compact subset of (R_1, R_2) . Then the zeros of $p_n(t, R)$ are increasing (respectively, decreasing) functions of $R \in (R_1, R_2)$ if $\frac{\partial}{\partial R} \log \omega(t; R)$ is an increasing (respectively, decreasing) function of t on $\mathcal{N}$.

We also need the following fundamental Bernstein–Widder theorem [46], which gives a necessary and sufficient condition for absolute monotonicity over $(-\infty, 0]$ via Laplace transform.

Theorem 3.4 (Bernstein–Widder [46]). *A function $F : (-\infty, 0] \rightarrow [0, +\infty)$ is absolutely monotonic on $(-\infty, 0]$ if and only if there exists a finite Borel measure μ supported on $[0, +\infty)$ such that*

$$F(x) = \int_0^\infty e^{xt} d\mu(t) \quad \text{for all } x \leq 0. \tag{3.22}$$

Note that the successive derivatives of F at zero are exactly the moments of the representing measure μ , i.e;

$$F^{(k)}(0) = \int_0^\infty t^k d\mu(t), \quad \text{for all } k \geq 0.$$

Therefore, these moments satisfy the following conditions derived by Stieltjes.

Theorem 3.5 (Stieltjes, [47]). *Let $(\lambda_0, \lambda_1, \dots, \lambda_p)$ be positive real numbers of the successive moments of a finite Borel measure on $[0, +\infty)$ if and only if all associated Hankel determinants are nonnegative*

$$H_{2s} = \begin{vmatrix} \lambda_0 & \lambda_1 & \cdots & \lambda_s \\ \lambda_1 & \lambda_2 & \cdots & \lambda_{s+1} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_s & \lambda_{s+1} & \cdots & \lambda_{2s} \end{vmatrix} \geq 0, \quad \text{for all } 2 \leq 2s \leq p,$$

and

$$H_{2s+1} = \begin{vmatrix} \lambda_1 & \lambda_2 & \cdots & \lambda_{s+1} \\ \lambda_2 & \lambda_3 & \cdots & \lambda_{s+2} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_{s+1} & \lambda_{s+2} & \cdots & \lambda_{2s+1} \end{vmatrix} \geq 0, \quad \text{for all } 3 \leq 2s+1 \leq p.$$

In particular, the 2×2 principal minors encode the inequality

$$\begin{vmatrix} F^{(k)}(0) & F^{(k+1)}(0) \\ F^{(k+1)}(0) & F^{(k+2)}(0) \end{vmatrix} = F^{(k)}(0)F^{(k+2)}(0) - (F^{(k+1)}(0))^2 \geq 0.$$

A shift in the function F provides us with the following corollary.

Corollary 3.1. *Let F be absolutely monotonic on $(-\infty, 0]$. Then the sequence $\{F^{(k)}(-R)\}$ is log-convex for any positive real number R , i.e;*

$$\left(F^{(k+1)}(-R)\right)^2 \leq F^{(k)}(-R) F^{(k+2)}(-R) \quad \text{for all } k \geq 0.$$

We are now in a position to prove the following.

Theorem 3.6. *Let F be an absolutely monotonic function over the interval $(-\infty, 0]$. Then, for any $k \geq 0$, the zeros of the orthogonal polynomial $\pi_k^F(.; R)$ are increasing functions of the parameter $R \in (0, \infty)$.*

Proof. The weight function

$$\omega(k; R) = \frac{F^{(k)}(-R)R^k}{k!}$$

is positive for any positive number R and with continuous partial derivative with respect to the parameter R in $[0, \infty)$. Moreover,

$$\frac{\partial}{\partial R} \log \omega(k; R) = \frac{F^{(k+1)}(-R)}{F^{(k)}(-R)} + \frac{k}{R}. \quad (3.23)$$

Using the log-convexity of Corollary 3.1, we conclude that $\frac{\partial}{\partial R} \log \omega(k; R)$ is an increasing function of R . We conclude the proof using Theorem 3.3. $\square$

3.3 Connection Between Optimal Threshold Factors and The Orthogonal Polynomials $\pi_k^F(\cdot; R)$

Let $\Lambda_{2p} = (\lambda_0, \lambda_1, \dots, \lambda_{2p-1})$ be a sequence of positive real numbers. Let F be any smooth function such that

$$F^{(k)}(0) = \lambda_k, \quad k = 0, 1, \dots, 2p-1. \quad (3.24)$$

From (3.11), the orthogonal polynomials $\pi_k^F(\cdot; R)$ associated with the measure μ_R^F , up to order p , depend only on the sequence Λ_{2p} . Therefore, these polynomials can be computed without explicitly knowing the function F itself. Since the measure is supported on the set of non-negative integers, all zeros of these orthogonal polynomials must be real and non-negative. Consequently, if for some positive real number R_0 , any of the polynomials $\pi_k^F(\cdot; R_0)$, $0 \leq k \leq p$, has a negative or non-real zero, then there does not exist an absolutely monotonic function F on the interval $[-R_0, 0]$ satisfying the conditions in (3.24). In particular, both the optimal threshold factor and the Bernstein constant must be less or equal to R_0 . To summarize

Theorem 3.7. *Given a sequence $\Lambda_{2p} = (\lambda_0, \lambda_1, \dots, \lambda_{2p-1})$ of positive real numbers. Let F be any smooth function that satisfies (3.24). Let R_0 be a positive real number. If any of the orthogonal polynomials $\pi_k^F(\cdot; R_0)$, $k = 1, 2, \dots, p$, has a negative or non-real zero then*

$$R_m(\Lambda_{2p}) \leq R_\infty(\Lambda_{2p}) \leq R_0.$$

Example 3.6. Consider the sequence $\Lambda_4 = (1, 1, 1, 0.5)$. From (3.11), the orthogonal polynomial $\pi_2^F(t; R)$ of degree 2 associated with the discrete measure μ_R^F is given by

$$\pi_2^F(t; R) = Rt^2 + t(0.5R^3 - 2R^2 - R) - 0.5R^4 + R^3.$$

The zeros of $\pi_2^F(t; R)$ are given by

$$\xi_1^F(R) = -0.25R^2 + R - \sqrt{0.0625R^4 - 0.25R^2 + R + 0.25} + 0.5,$$

$$\xi_2^F(R) = -0.25R^2 + R + \sqrt{0.0625R^4 - 0.25R^2 + R + 0.25} + 0.5.$$

As can be seen from Figure 3.1, the zeros of $\pi_2(\cdot; R)$ are non-negative for $R \leq 2$ and the smallest zero becomes negative for $R > 2$, signaling the breakdown of positivity of the associated measure. Therefore, we can conclude that, for any $\epsilon > 0$, there is no absolutely monotonic function F over the interval $[-2 - \epsilon, 0]$ such that

$$F(0) = F'(0) = F''(0) = 1 \quad \text{and} \quad F^{(3)}(0) = 0.5. \quad (3.25)$$

In fact it can be shown using Bernstein's theory in [32] that the polynomial

$$F(x) = \frac{1}{3} + \frac{2}{3} \left(1 + \frac{x}{2}\right)^3$$

is the unique function that is absolutely monotonic over the interval $[-2, 0]$ and satisfies

(3.25). Therefore, we have

$$R_m(\Lambda_4) = R_\infty(\Lambda_4) = 2 \quad \text{for any } m \geq 3.$$

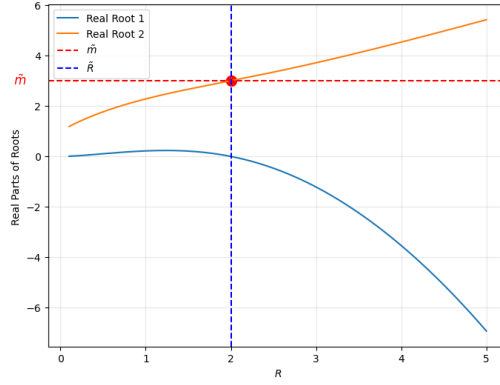


Figure 3.1: Roots of the orthogonal polynomial $\pi_2^F(t; R)$ as a function of R . The vertical red line indicates the critical value $\tilde{R} = 2$, where the smallest root vanishes.

CHAPTER 4

DISCRETE ORTHOGONAL POLYNOMIALS AND SHARP BOUNDS FOR THE OPTIMAL THRESHOLD FACTORS

In this chapter, we employ the discrete orthogonal polynomials, defined in the previous chapter, to derive sharp bounds for the optimal threshold factor. The upper bound is established by comparing the nodes of positive quadrature formulas with integer nodes to those of the Gaussian quadrature associated with the discrete measure. This leads to precise bounds for the optimal threshold factors for generalized Poisson-Charlier sequences in terms of the smallest zero of generalized Laguerre polynomials; and for Meixner sequences in terms of the smallest zero of non-standard Jacobi polynomials.

This chapter is organized as follows. In Section 4.1, we establish a general comparison theorem between arbitrary positive quadrature rules and Gaussian quadrature associated with a given positive measure possessing finite moments of all orders. This result is then employed to derive an upper bound for the optimal threshold factor of sequences exhibiting specific structural properties. In Section 4.2, we employ duality

arguments to obtain a lower bound for the optimal threshold factors. Applications to generalized Poisson-Charlier and Meixner sequences are presented in Section 4.3.

4.1 Positive Quadrature and Upper Bound for the Optimal Threshold Factor $R_m(\Lambda_{2p})$

The idea behind the upper bound is to compare Gaussian quadrature with respect to the measure μ_R^F and the quadrature defined in (3.2). We first prove the following theorem which roughly states that the largest zero of an orthogonal polynomial is an upper bound for the nodes of any positive quadrature. More precisely, let μ be a finite positive measure on the real line, possessing finite moments of all orders and having infinitely many points of increase. Let $\pi_1, \pi_2, \dots, \pi_p, \dots$ denote the sequence of monic orthogonal polynomials with respect to μ . We denote by $\mathbb{P}_p$ the space of all polynomials of degree at most p .

Theorem 4.1. *Given a positive quadrature rule with respect to the measure μ which is exact in $\mathbb{P}_{2p-1}$,*

$$\int P(t) d\mu = \sum_{k=1}^s \beta_k P(\rho_k) \quad \text{for any } P \in \mathbb{P}_{2n-1}, \quad (4.1)$$

with $s \geq p$, $0 \leq \rho_1 < \rho_2 < \dots < \rho_s$ and $\beta_j > 0, j = 1, 2, \dots, s$. Then $\rho_s \geq t_p$ and $\rho_1 \leq t_1$ where $t_1 < t_2 < \dots < t_p$ are the zeros of the orthogonal polynomial π_p . Moreover, $\rho_s = t_p$ if and only if the quadrature (4.1) coincides with the Gaussian quadrature with respect to the measure μ .

Proof. Consider the polynomial

$$Q(t) := \pi_p(t) \frac{\pi_p(t)}{t - t_p} = (t - t_p) \prod_{i=1}^{p-1} (t - t_i)^2. \quad (4.2)$$

Applying (4.1) and invoking orthogonality, we obtain

$$\int Q(t) d\mu = - \sum_{k=1}^s \beta_k (t_1 - \rho_k)^2 \dots (t_{p-1} - \rho_k)^2 (t_p - \rho_k) = 0. \quad (4.3)$$

Since $s \geq p$, we conclude that there exists an integer $k \in \{1, 2, \dots, s\}$ such that $\rho_k \geq t_p$. In particular, we have $\rho_s \geq t_p$. If $\rho_s = t_p$ then from (4.3) we remark that for $k = 1, 2, \dots, s-1$, $(\rho_k - t_1) \dots (\rho_k - t_{p-1}) = 0$. In other words, $\rho_1, \rho_2, \dots, \rho_{s-2}$ and ρ_{s-1} are zeros of the polynomial $\psi(t) = (t - t_1)(t - t_2) \dots (t - t_{p-1})$. Thus, we necessarily have $s - 1 = p - 1$ and $\rho_k = t_k$ for $k = 1, 2, \dots, p - 1$. Therefore, the quadrature (4.1) coincides with the Gaussian quadrature. To prove that $t_1 \geq \rho_1$ we proceed as follows.

Define the polynomial

$$S(t) = \pi_p(t) \frac{\pi_p(t)}{t - t_1} = (t - t_1) \prod_{i=2}^p (t - t_i)^2.$$

Applying (4.1) and invoking orthogonality, we obtain

$$\int S(t) d\mu = - \sum_{k=1}^s \beta_k (t_2 - \rho_k)^2 \dots (t_p - \rho_k)^2 (t_1 - \rho_k) = 0.$$

Therefore, there exists an integer $k \in \{1, 2, \dots, s\}$ such that $\rho_k \leq t_1$. In particular,

we have $\rho_1 \leq t_1$.

□

Definition 4.1. A sequence $\Lambda_p = (\lambda_1, \lambda_2, \dots, \lambda_p)$ is said to be absolutely positive if there exists a function F absolutely monotonic on $(-\infty, 0]$ such that $F^{(k)}(0) = \lambda_k$ for $k = 0, 1, \dots, p$.

Theorem 4.2. Let $\Lambda_{2p} = (\lambda_1, \lambda_2, \dots, \lambda_{2p-1})$ be an absolutely positive sequence. Then, the zeros of the degree p orthogonal polynomial $\pi_p^F(\cdot; R)$ are nonnegative for any $R > 0$, increasing as a function of R and such that the largest zero diverges to infinity as R goes to infinity.

Proof. That the zeros of $\pi_p^F(\cdot; R)$ are nonnegative and are increasing functions with respect to R is a consequence of Theorem 3.6. We prove that the largest zero of $\pi_p^F(\cdot; R)$ diverges to infinity as R goes to infinity by induction on p . For $p = 1$, we have

$$\pi_1^F(x; R) = x - \frac{\lambda_2}{\lambda_1}R.$$

The only zero is given by $\xi_1^F(R) = \frac{\lambda_2}{\lambda_1}R$ and satisfies $\lim_{R \rightarrow \infty} \xi_1^F(R) = \infty$. Assume the hypothesis to be true for any $k \leq p-1$. Let $\xi_{p-1}^F(R)$ and $\xi_p^F(R)$ the largest zero of $\pi_{p-1}^F(\cdot; R)$ and $\pi_p^F(\cdot; R)$ respectively. According to the alternation theorem of the zeros of orthogonal polynomials, we have

$$\xi_{p-1}^F(R) < \xi_p^F(R).$$

Therefore, $\lim_{R \rightarrow \infty} \xi_p^F(R) = \infty$.

□

A direct consequence of the previous theorem is the following upper bound for the optimal threshold factors.

Theorem 4.3. *Given an absolutely positive sequence Λ_{2p} and let $\bar{R}$ be the unique positive real number such that the largest zeros of $\pi_p^F(\cdot; \bar{R})$ is equal m . Then*

$$R_m(\Lambda_{2p}) \leq \bar{R}.$$

Equality is attained when all zeros of $\pi_p^F(\cdot; \bar{R})$ are nonnegative integers. In this case, the optimal threshold polynomial is given by

$$\Phi(\Lambda_{2p})(x) = \sum_{i=1}^p \omega_i \left(1 + \frac{x}{\bar{R}}\right)^{\xi_i^F},$$

where $\xi_1^F < \xi_2^F, \dots < \xi_p^F$, are the zeros of the orthogonal polynomial $\pi_p^F(\cdot; \bar{R})$ and $\omega_i, i = 1, \dots, p$ are the weights of the Gaussian quadrature associated with the measure $\mu_{\bar{R}}^F$.

Proof. According to Remark 2.3, the optimal threshold factor $R_m(\Lambda_{2p})$ is the largest positive real number R such that the measure μ_R^F admits a positive quadrature with integer nodes not exceeding m , and is exact for all polynomials of degree at most $2p - 1$. If $R_m(\Lambda_{2p}) < \bar{R}$ and since the zeros of the orthogonal polynomial $\pi_p^F(\cdot; R)$ are strictly increasing function of R , we would have $\xi_p^F < m$, which contradicts the statement of Theorem 4.1. The implications of the equality case stem from the fact that it yields a positive quadrature rule with integer nodes, all of which are less than or equal to m . □

Example 4.1. Consider the sequence

$$\Lambda_4 = (1, 0.25, 0.3125, 0.7031).$$

Using Proposition 4.3, we provide an upper bound for the optimal threshold factor $R_{10}(\Lambda_4)$. For each $R > 0$, the moments associated with the discrete measure μ_R^F are given by

$$m_0 = 1, \quad m_1 = R, \quad m_2 = 0.3125R^2 + 0.25R, \quad m_3 = 0.7031R^3 + 3R^2 + R.$$

Using these moments, the orthogonal polynomial of degree 2 is constructed via (3.11) and is given by

$$\pi_2^F(t; R) = (0.25R^2 + 0.25R)t^2 + (-0.6250R^3 - 0.8750R^2 - 0.2500R)t + (0.0781R^4 + 0.0781R^3).$$

Solving for the roots of $\pi_2^F(t; R)$, we obtain the real-valued functions $\xi_1^F(R)$ and $\xi_2(R)$, both of which are nonnegative and strictly increasing in R (see Figure 4.1). Explicit expressions of the zeros are

$$\xi_1(R) = \frac{1.25R^2 + 1.75R - 2\sqrt{0.3125R^4 + 0.9375R^3 + R^2 + 0.4375R + 0.0625} + 0.5}{R + 1},$$

$$\xi_2(R) = \frac{1.25R^2 + 1.75R + 2\sqrt{0.3125R^4 + 0.9375R^3 + R^2 + 0.4375R + 0.0625} + 0.5}{R + 1}.$$

Numerical evaluation shows that the largest root $\xi_2(\tilde{R})$ reaches $m = 10$ when $\tilde{R} = 3.7626$. Therefore, according to Theorem 4.3, an upper bound for the optimal threshold

factor is

$$R_m(\Lambda_4) \leq 3.7626,$$

Using the algorithm of Chapter 2, the exact value of the optimal threshold factor is given by $R_m(\Lambda_4) = 3.5557$

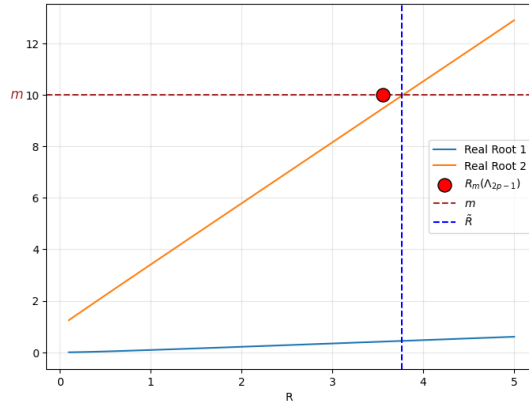


Figure 4.1: Roots of the orthogonal polynomial $\pi_2^F(t; R)$ as functions of R . The vertical blue line indicates the value $\tilde{R}$ at which the largest root $\xi_2(R)$ is equal to $m = 10$.

4.2 Lower Bound for $R_m(\Lambda_{2p})$

This section establishes a lower bound for the optimal threshold factor $R_m(\Lambda_{2p})$ using duality arguments.

We need the following Farkas lemma.

Lemma 4.1 (Farkas' Lemma, [48]). *Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ and $\mathbf{b} \in \mathbb{R}^m$. Then exactly one of the following two assertions holds*

1. There exists a vector $\mathbf{x} \in \mathbb{R}^n$ such that

$$\mathbf{Ax} = \mathbf{b} \quad \text{and} \quad \mathbf{x} \geq 0.$$

2. There exists a vector $\mathbf{y} \in \mathbb{R}^m$ such that

$$\mathbf{A}^\top \mathbf{y} \geq 0 \quad \text{and} \quad \mathbf{b}^\top \mathbf{y} < 0.$$

Here, the notation $\mathbf{x} \geq 0$ means that all components of the vector $\mathbf{x}$ are non-negative.

Using Farkas's Lemma we establish the following.

Theorem 4.4. *let $\Lambda_{p+1} = (\lambda_0, \dots, \lambda_p)$ be a sequence of positive real number and $m \geq p$. A real number $\bar{R} > 0$ satisfies*

$$\bar{R} \leq R_m(\Lambda_{p+1})$$

if and only if for any polynomial P of degree at most p satisfying

$$P(j) \geq 0 \quad \text{for } j = 0, 1, \dots, m, \tag{4.4}$$

we have

$$\int P(t) d\mu_{\bar{R}}(t) \geq 0. \tag{4.5}$$

Proof. Let $\bar{R}$ be a real number such that $\bar{R} \leq R_m(\Lambda_{p+1})$. According to Remark 2.3,

we have a positive quadrature with integer nodes smaller than m , that is there exist non-negative real numbers α_i and integers $m_i \leq m, i = 1, \dots, s$ such that

$$\int P(t) d\mu_R^F = \sum_{i=1}^s \alpha_i P(m_i) \quad \text{for any } P \in \mathbb{P}_p. \quad (4.6)$$

Therefore, using the condition (4.4), we conclude that (4.5) holds for any polynomial P of degree at most p satisfying (4.4). Conversely, let us assume that $\bar{R}$ is such that, for any polynomial P of degree at most p such that $P(j) \geq 0$ for $j = 0, 1, \dots, m$, we have $\int P(t) d\mu_R^F(t) \geq 0$. Expressing P in the monomial basis as $P(t) = \sum_{k=0}^p \gamma_k t^k$ and set $\gamma : (\gamma_0, \gamma_1, \dots, \gamma_p)^T$ and A the $(p+1, m+1)$ matrix $A = (a_{ij})$ with $a_{ij} = j^i$ for $i = 0, 1, \dots, p$ and $j = 0, 1, \dots, m$. Clearly, we have $\gamma^T A = (P(0), P(1), \dots, P(m))$. Moreover, if we denote by $b = (B_0(\Lambda_{p+1}, R), B_1(\Lambda_{p+1}, R), \dots, B_p(\Lambda_{p+1}, R))^T$. Using (4.6), we obtain $\gamma^T b = \int P(t) d\mu_R^F(t)$. Therefore, for any $\gamma \in \mathbb{R}^{n+1}$ such that $\gamma^T A \geq 0$ we have $\gamma^T b \geq 0$. Thus, by Farkas' Lemma 4.1, there exists a vector $\alpha = (\alpha_0, \alpha_1, \dots, \alpha_m)^T \geq 0$ such that $A\alpha = b$, which in turn is equivalent to the representation of the polynomial $\mathcal{H}_p(\cdot; \bar{R})$ as

$$\mathcal{H}_p(x; \bar{R}) = \sum_{k=0}^m \alpha_k (x - k)^p.$$

Therefore, $\bar{R} \leq R_{m,n}$. This concludes the proof. $\square$

Definition 4.2. A non-zero real polynomial P is said to be admissible if it is nonnegative over the integers, i.e.;

$$P(j) \geq 0 \quad \text{for all } j \in \mathbb{Z}.$$

Define the following parameter

$$\tau_p^F = \sup_{R>0} \sup_{P \in \mathcal{C}_p} \left(\frac{\int t P(t) d\mu_R^F}{\int P(t) d\mu_R^F} - \xi_{p,p}^F \right), \quad (4.7)$$

where $\mathcal{C}_p$ denotes the set of all admissible polynomials of degree at most $2(p-1)$, and $\xi_{p,p}^F$ is the largest root of the orthogonal polynomial $\pi_p^F(\cdot; R)$ with respect to the measure μ_R^F .

Generalizing the techniques of [36], we can show the following lower bound for $R_m(\Lambda_{2p})$ in terms of τ_p^F

Theorem 4.5. *Given an absolutely positive sequence Λ_{2p} and let $\bar{R}$ be the unique positive real number such that the largest zeros of $\pi_p^F(\cdot; \bar{R})$ is equal to $m - \tau_p^F$. Then*

$$R_m(\Lambda_{2p}) \geq \bar{R}.$$

Our goal in the remainder of this section is to establish the inequality $\tau_p^F \leq p-1$.

Given an admissible polynomial P , we define the modified measure

$$\bar{\mu}_R^F = \sum_{j=0}^{\infty} \frac{F^{(j)}(-R) R^j P(j)}{j!} \delta_j.$$

To establish an upper bound for τ_p^F , we start by establishing the following.

Proposition 4.1. *Let P be an admissible polynomial. Denotes $\bar{\xi}_1$ the zero of the*

degree 1 orthogonal polynomial $\Pi_1(\cdot; R)$ associated with the measure

$$\bar{\mu}_R^{F(1)} = \sum_{j=0}^{\infty} \frac{F^{(j+1)}(-R)R^j P(j)}{j!} \delta_j,$$

and $\bar{\xi}_1^+$ the zero of the degree 1 orthogonal polynomial $\Pi_1^+(\cdot; R)$ with respect to the measure

$$\bar{\mu}_R^{F^+} = \sum_{j=0}^{\infty} \frac{F^{(j)}(-R)R^j P^+(j)}{j!} \delta_j, \quad \text{where } P^+(t) := P(t-1).$$

Then the following inequality holds

$$\bar{\xi}_1^+ \leq \bar{\xi}_1 + 1.$$

Proof. Define the polynomial

$$G_1(x) = \int (x-t) d\bar{\mu}_R^{F(1)}(t) = \omega_1(x - \bar{\xi}_1). \quad (4.8)$$

Clearly, $G_1(\bar{\xi}_1) = 0$. Therefore, there exists a constant ω_1 such that

$$G_1(x) = \omega_1(x - \bar{\xi}_1). \quad (4.9)$$

Define the polynomial

$$G_2(x) = \int (x-t)^2 d\bar{\mu}_R^{F^+}(t). \quad (4.10)$$

Using (3.7), the polar form g_2 of $G_2(x)$ satisfies

$$\begin{aligned} g_2(0, x) &= - \int t(x-t) d\bar{\mu}_R^{F^+}(t) = -R \int (x-(t+1)) d\bar{\mu}_R^{F^{(1)}}(t) \\ &= -R \int ((x-1)-t) d\bar{\mu}_R^{F^{(1)}}(t) = -RG_1(x-1). \end{aligned}$$

Using 4.9, we observe that $g_2(0, \bar{\xi}_1 + 1) = 0$. Hence, there exist constants α_0 and α_1 such that

$$G_2(x) = \alpha_0 x^2 + \alpha_1 (x - (\bar{\xi}_1 + 1))^2. \quad (4.11)$$

Since

$$\begin{aligned} G_2(0) &= \int t^2 d\bar{\mu}_R^{F^+}(t) = \alpha_1 (\bar{\xi}_1 + 1)^2 \geq 0, \\ G_2(\bar{\xi}_1 + 1) &= \int (\bar{\xi}_1 + 1 - t)^2 d\bar{\mu}_R^{F^+}(t) = \alpha_0 (\bar{\xi}_1 + 1)^2 \geq 0, \end{aligned}$$

we conclude that the constants α_0, α_1 are nonnegative. Differentiating both (4.10) and (4.11) with respect to x , and applying Gauss quadrature, we obtain

$$\gamma_1(x - \bar{\xi}_1^+) = \alpha_0 x + \alpha_1 (x - (\bar{\xi}_1 + 1)), \quad (4.12)$$

with $\gamma_1 > 0$. Evaluating both sides of (4.12) at $x = \bar{\xi}_1^+$ gives the desired result $\bar{\xi}_1^+ \leq \bar{\xi}_1 + 1$. $\square$

By orthogonality with respect to $\bar{\mu}_R^{F^{(1)}}$, the unique zero $\bar{\xi}_1$ of the polynomial

$\Pi_1^{F(1)}(\cdot; R)$ satisfies

$$\int (t - \bar{\xi}_1) d\bar{\mu}_R^{F(1)}(t) = \int (t - \bar{\xi}_1) P(t) d\mu_R^{F(1)}(t) = 0.$$

Thus,

$$\bar{\xi}_1 = \frac{\int t P(t) d\mu_R^{F(1)}(t)}{\int P(t) d\mu_R^{F(1)}(t)}.$$

Similarly, we have

$$\bar{\xi}_1^+ = \frac{\int t P(t-1) d\mu_R^{F(1)}(t)}{\int P(t-1) d\mu_R^{F(1)}(t)}.$$

Therefore, Proposition 4.1 can be re-stated as

Corollary 4.1. *For any admissible polynomial P and any positive real number R , the following inequality holds.*

$$\frac{\int t P(t) d\mu_R^F(t)}{\int P(t) d\mu_R^F(t)} \leq \frac{\int t P(t+1) d\mu_R^{F(1)}(t)}{\int P(t+1) d\mu_R^{F(1)}(t)} + 1.$$

Iterating the previous inequality leads to the following.

Corollary 4.2. *For any admissible polynomial P and any non-negative integer k , the following inequality holds.*

$$\frac{\int t P(t) d\mu_R^F(t)}{\int P(t) d\mu_R^F(t)} \leq \frac{\int t P(t+k) d\mu_R^{F(k)}(t)}{\int P(t+k) d\mu_R^{F(k)}(t)} + k. \quad (4.13)$$

We shall need the following proposition.

Proposition 4.2. *Let F be absolutely monotonic on $(-\infty, 0]$ and $R > 0$. Then, for*

any admissible polynomial P , we have

$$\frac{\int t P(t) d\mu_R^{F^{(1)}}(t)}{\int P(t) d\mu_R^{F^{(1)}}(t)} \leq \frac{\int t P(t) d\mu_R^F(t)}{\int P(t) d\mu_R^F(t)}. \quad (4.14)$$

Proof. Using the definition of the measures μ_R^F and $\mu_R^{F^{(1)}}$, we have

$$\int t P(t) d\mu_R^{F^{(1)}} \int P(t) d\mu_R^F = \sum_{j,k=0}^{\infty} \frac{j P(j) P(k) F^{(j+1)}(-R) F^{(k)}(-R) R^{j+k}}{j! k!},$$

and similarly,

$$\int t P(t) d\mu_R^F \int P(t) d\mu_R^{F^{(1)}} = \sum_{j,k=0}^{\infty} \frac{j P(j) P(k) F^{(j)}(-R) F^{(k+1)}(-R) R^{j+k}}{j! k!}.$$

Thus, the difference is given by

$$\begin{aligned} & \left(\int t P(t) d\mu_R^{F^{(1)}} \right) \left(\int P(t) d\mu_R^F \right) - \left(\int t P(t) d\mu_R^F \right) \left(\int P(t) d\mu_R^{F^{(1)}} \right) \\ &= \sum_{j,k=0}^{\infty} \frac{j P(j) P(k) R^{j+k}}{j! k!} \begin{vmatrix} F^{(k)}(-R) & F^{(k+1)}(-R) \\ F^{(j)}(-R) & F^{(j+1)}(-R) \end{vmatrix} \\ &= \sum_{m=0}^{\infty} \sum_{j=0}^m \frac{j P(j) P(m-j)}{j! (m-j)!} \begin{vmatrix} F^{(m-j)}(-R) & F^{(m-j+1)}(-R) \\ F^{(j)}(-R) & F^{(j+1)}(-R) \end{vmatrix} R^m. \end{aligned}$$

Corollary 3.1 ensures the log-convexity condition

$$F^{(j)}(-R) F^{(m-j+1)}(-R) \geq F^{(j+1)}(-R) F^{(m-j)}(-R), \quad j \leq m-j,$$

which in turns ensures the non-negativity of the sum. This concludes the proof. $\square$

From the previous proposition, we can easily deduce the following.

Corollary 4.3. *Let F be absolutely monotonic on $(-\infty, 0]$ and $R > 0$. Then, for every admissible polynomial P and for any integer h , we have*

$$\frac{\int t P(t) d\mu_R^{F(h)}(t)}{\int P(t) d\mu_R^{F(h)}(t)} \leq \frac{\int t P(t) d\mu_R^F(t)}{\int P(t) d\mu_R^F(t)}. \quad (4.15)$$

Before providing the main result, we state the following result proved in [36].

Proposition 4.3 ([36]). *Let P be an admissible polynomial of degree at most $2p - 2$.*

The polynomial

$$Q(t) = \sum_{k=0}^{p-1} \binom{p-1}{k}^2 P(t+k) \quad (4.16)$$

satisfies $Q(t) \geq 0$ for all $t \in \mathbb{R}$.

Theorem 4.6. *For a given absolutely positive sequence Λ_{2p} the parameter τ_p^F , defined in (4.7) satisfies the inequality*

$$\tau_p^F \leq p - 1 \quad \text{for any } p \geq 2.$$

Proof. Let $R > 0$ be a fixed real number, and let $P \in \mathcal{C}_p$ be an admissible polynomial of degree at most $2(p-1)$. By Proposition 4.3, the degree $2p-2$ polynomial Q defined in (4.16) is non-negative over the whole real line. By Gauss quadrature, we have

$$\begin{aligned} \int t Q(t) d\mu_R^F &= \sum_{k=1}^p \alpha_k \xi_{k,p}^F(R) Q(\xi_{k,p}^F(R)) \\ &\leq \xi_{p,p}^F(R) \sum_{k=1}^p \alpha_k Q(\xi_{k,p}^F(R)) = \xi_{p,p}^F(R) \int Q(t) d\mu_R^F. \end{aligned}$$

From the expression of the polynomial Q , the previous inequality can be written as

$$\sum_{k=0}^{p-1} \binom{p-1}{k}^2 \int P(t+k) d\mu_R^F \leq \xi_{p,p}^F \sum_{k=0}^{p-1} \binom{p-1}{k}^2 \int P(t+k) d\mu_R^F.$$

Therefore, there exists an index $j \in \{0, \dots, p-1\}$ such that

$$\frac{\int t P(t+j) d\mu_R^F}{\int P(t+j) d\mu_R^F} \leq \xi_{p,p}^F(R). \quad (4.17)$$

Thus, from inequality (4.15), we have

$$\frac{\int t P(t+j) d\mu_R^{F(j)}}{\int P(t+j) d\mu_R^{F(j)}} \leq \xi_{p,p}^F(R).$$

Therefore, using (4.13), we obtain

$$\frac{\int t P(t) d\mu_R^F}{\int P(t) d\mu_R^F} \leq \xi_{p,p}^F(R) + j \leq \xi_{p,p}^F(R) + p - 1. \quad (4.18)$$

This concludes the proof by invoking the definition of τ_p^F . $\square$

Using the bound $\tau_p^F \leq p - 1$ along with Theorems 4.5, we obtain the following bounds on the optimal threshold factors.

Theorem 4.7. *Let $m, p \in \mathbb{N}$ with $m \geq 2p - 1$ and let $\Lambda_{2p} = (\lambda_0, \dots, \lambda_{2p-1})$ be an absolutely positive sequence. Let R_{min} and R_{max} the unique positive real numbers such that*

$$\xi_{p,p}^F(R_{max}) = m, \quad \xi_{p,p}^F(R_{min}) = m - p + 1.$$

Then, the following bound for the optimal threshold factor

$$R_{min} \leq R_m(\Lambda_{2p+1}) \leq R_{max}$$

holds.

4.3 Bounds on the Optimal threshold Factors of Some Classical Sequences

As an application of Theorem 4.7, this section presents sharp bounds for the optimal threshold factors associated with the sequences

$$\Lambda_{2p}(\gamma) = (1, \gamma, \gamma^2, \dots, \gamma^{2p-1}) \quad \text{with } \gamma > 0,$$

and

$$\Lambda_{2p}(\beta) = (1, \beta^{(1)}, \beta^{(2)}, \dots, \beta^{(2p-1)}) \quad \text{with } \beta > 0.$$

We begin by establishing that both sequences are absolutely positive and correspond, respectively, to the functions $F(x) = e^{\gamma x}$ and $G(x) = (1-x)^{-\beta}$. The orthogonal polynomials associated with $\Lambda_{2p}(\gamma)$ are identified as generalized Poisson–Charlier polynomials, while those associated with $\Lambda_{2p}(\beta)$ correspond to Meixner orthogonal polynomials. Accordingly, we shall refer to the former as Generalized Poisson–Charlier sequences and the latter as Meixner sequences. The resulting bounds on the optimal threshold factors will be expressed in terms of the smallest zeros of generalized

Laguerre polynomials for the sequence $\Lambda_{2p}(\gamma)$, and in terms of the smallest zero of Jacobi-like orthogonal polynomials for the sequence $\Lambda_{2p}(\beta)$.

Many classical orthogonal polynomials can be expressed in terms of hypergeometric functions. The general form of the hypergeometric function is defined by

$${}_pF_q \left(\begin{matrix} a_1, a_2, \dots, a_p \\ b_1, b_2, \dots, b_q \end{matrix} ; t \right) = \sum_{n=0}^{\infty} \frac{(a_1)_n (a_2)_n \cdots (a_p)_n}{(b_1)_n (b_2)_n \cdots (b_q)_n} \frac{t^n}{n!}, \quad (4.19)$$

where the Pochhammer symbol (rising factorial) is defined by [49]

$$(a)_n = a(a+1)(a+2) \cdots (a+n-1) = \frac{\Gamma(a+n)}{\Gamma(a)}. \quad (4.20)$$

A special case of this is the *Gauss hypergeometric function*,

$${}_2F_1 \left(\begin{matrix} a, b \\ c \end{matrix} ; t \right) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{t^n}{n!}, \quad (4.21)$$

which converges for $|t| < 1$.

Of particular interest to us in this section are the Jacobi polynomials expressed in terms of hypergeometric functions as

$$P_p^{(\alpha, \beta)}(t) = \frac{(\alpha+1)_p}{p!} {}_2F_1 \left(\begin{matrix} -p, p+\alpha+\beta+1 \\ \alpha+1 \end{matrix} ; \frac{1-t}{2} \right). \quad (4.22)$$

are orthogonal with respect the the weight function $\omega_{\alpha, \beta}(t) = (1-t)^\alpha (1+t)^\beta$ over the

interval $[-1, 1]$ when $\alpha, \beta > -1$, i.e.;

$$\int_{-1}^1 P_i^{(\alpha, \beta)}(t) P_j^{(\alpha, \beta)}(t) \omega_{\alpha, \beta}(t) dt = 0 \quad \text{if } i \neq j.$$

We also need the generalized Laguerre polynomials defined in terms of hypergeometric functions as

$$L_p^{(\alpha)}(t) = \frac{(\alpha + 1)_p}{p!} {}_1F_1 \left(\begin{matrix} -p \\ \alpha + 1 \end{matrix} ; t \right), \quad (4.23)$$

where $\alpha > -1$. They are orthogonal with respect to the weight function $\omega_\alpha(t) = t^\alpha e^{-t}$ over the interval $[0, \infty)$, that is

$$\int_0^\infty L_i^{(\alpha)}(t) L_j^{(\alpha)}(t) \omega_\alpha(t) dt = 0 \quad \text{if } i \neq j.$$

4.3.1 Bound on the optimal threshold factors of the generalized Poisson-Charlier sequence $\Lambda_{2p}(\gamma)$

The elements of the sequence $\Lambda_{2p}(\gamma)$ are the values of the successive derivatives of the function $F(x) = e^{\gamma x}$ at the origin. Therefore, the sequence is associated with the generalized Poisson-Charlier measure defined by (3.8). The corresponding orthogonal polynomials are the generalized Poisson-Charlier orthogonal polynomial given in terms of hypergeometric function as

$$C_p^\gamma(t; R) = {}_2F_0 \left(\begin{matrix} -p, -t \\ - \end{matrix} ; -\frac{1}{\gamma R} \right).$$

Since the function F is absolutely monotonic on the interval $(-\infty, 0]$, it follows from Theorem 3.6 that the zeros of the associated orthogonal polynomial $C_p^\gamma(t; R)$ increase monotonically with respect to the parameter R . Furthermore, it is well known that these zeros diverge to infinity as $R \rightarrow \infty$. Consequently, the sequence $\Lambda_{2p}(\gamma)$ is absolutely positive.

Let R_{min} and R_{max} the unique positive real numbers such that

$$\xi_{p,p}^F(R_{max}) = m, \quad \xi_{p,p}^F(R_{min}) = m - p + 1,$$

where $\xi_{p,p}^F$ is the largest zero of the polynomial $C_p(\cdot; R)$. From the relation

$$C_p^\gamma(t; R) = p! L_p^{(t-p)}(\gamma R), \quad (4.24)$$

we conclude that R_{max} and R_{min} satisfy

$$L_p^{(m-p)}(\gamma R_{max}) = 0 \quad \text{and} \quad L_p^{(m-2p+1)}(\gamma R_{max}) = 0. \quad (4.25)$$

Moreover, since the zeros of the generalized Poisson–Charlier polynomials increase monotonically with respect to the parameter γ , the quantities R_{min} and R_{max} represent the smallest values of R for which condition (4.25) is satisfied. This leads us to the following theorem.

Theorem 4.8. *For any integers m, p such that $m \geq 2p - 1$, the optimal threshold*

factor of the sequence $\Lambda_{2p}(\gamma) = (1, \gamma, \gamma^2, \dots, \gamma^{2p-1})$, $\gamma > 0$ satisfy

$$\frac{\ell_p^{(m-2p+1)}}{\gamma} \leq R_m(\Lambda_{2p}(\gamma)) \leq \frac{\ell_p^{(m-p)}}{\gamma},$$

where $\ell_p^{(\alpha)}$ refers to the smallest zero of the generalized Laguerre polynomial $L_p^{(\alpha)}$.

The upper and lower bounds for $R_m(\Lambda_{2p}(\gamma))$ established in Theorem 4.8 are presented in the table below for various values of p, m and for $\gamma = 0.5$ and 10. The exact values of the corresponding optimal threshold factors are computed using the algorithm outlined in Section 2.5.

p	Lower Bound	$R_m(\Lambda_{2p})$	Upper Bound
2	4.0000	$R_5(\Lambda_4) = 5.3013$	5.5279
3	0.8315	$R_5(\Lambda_6) = 2.0032$	3.0348
2	7.1010	$R_7(\Lambda_4) = 8.5758$	8.7085
3	3.0348	$R_7(\Lambda_6) = 5.3143$	5.5929
2	8.7084	$R_8(\Lambda_4) = 10.2143$	10.3431
3	4.2824	$R_8(\Lambda_6) = 6.7704$	6.9528

Table 4.1: Bounds for $R_m(\Lambda_{2p}(\gamma))$ with $\gamma = 0.5$

p	Lower Bound	$R_m(\Lambda_{2p})$	Upper Bound
2	0.2000	$R_5(\Lambda_4) = 0.2651$	0.2764
3	0.0416	$R_5(\Lambda_6) = 0.1000$	0.1517
2	0.3551	$R_7(\Lambda_4) = 0.4288$	0.4354
3	0.1517	$R_7(\Lambda_6) = 0.2651$	0.2797
2	0.4354	$R_8(\Lambda_4) = 0.5107$	0.5172
3	0.2141	$R_8(\Lambda_6) = 0.3373$	0.3476

Table 4.2: Bounds for $R_m(\Lambda_{2p}(\gamma))$ with $\gamma = 10$

4.3.2 Bound on the optimal threshold factors of the Meixner sequence $\Lambda_{2p}(\beta)$

The elements of the sequence $\Lambda_{2p}(\beta)$ are the values of the successive derivatives of the function $F(x) = (1-x)^{-\beta}$ at the origin. Therefore, the sequence is associated with the Meixner measure defined in by (3.9). The corresponding orthogonal polynomials are The Meixner polynomials given in terms of hypergeometric function as

$$M_p(t; \beta, R) = {}_2F_1 \left(\begin{matrix} -p, -t \\ \beta \end{matrix} ; 1 - \frac{1}{c} \right),$$

where $\beta > 0$, $0 < c < 1$ and $c = R/(1+R)$.

Since the function F is absolutely monotonic on the interval $(-\infty, 0]$, it follows from Theorem 3.6 that the zeros of the associated orthogonal polynomial $M_p(t; \beta, R)$ increase monotonically with respect to the parameter R . Furthermore, it is well known [45] that these zeros diverge to infinity as $R \rightarrow \infty$. Consequently, the sequence $\Lambda_{2p}(\gamma)$ is absolutely positive.

Let R_{min} and R_{max} the unique positive real numbers such that

$$\xi_{p,p}^F(R_{max}) = m, \quad \xi_{p,p}^F(R_{min}) = m - p + 1,$$

where $\xi_{p,p}^F$ is the largest zero of the polynomial $M_p(., \beta, R)$. From the relation between

Meixner and Jacobi polynomials [Nikiforov et al., [50]]

$$M_p(t; \beta, R) = p! \left(1 - \frac{1}{c}\right)^p P_p^{(t-p, -\beta-t-p)}\left(\frac{1+c}{1-c}\right), \quad (4.26)$$

we conclude that R_{max} and R_{min} satisfy

$$P_p^{(m-p, -\beta-m-p)}(1 + 2R_{max}) = 0 \quad \text{and} \quad P_p^{(m-2p+1, -\beta-m-1)}(1 + 2R_{min}) = 0. \quad (4.27)$$

Since the zeros of Meixner polynomials are increasing functions of the parameter R , The quantities R_{min} and R_{max} represent the smallest values of R for which condition (4.27) is satisfied. Note that the parameters β of the Jacobi polynomials in (4.27) is not grater than -1 . Therefore, these polynomials are not the classical Jacobi polynomials and are called *non-standard* Jacobi polynomials [51] and all their zeros real and larger than one [52]. This leads to the following theorem.

Theorem 4.9. *For any integers m, p such that $m \geq 2p - 1$, the optimal threshold factor of the sequence $\Lambda_{2p}(\beta) = (1, \beta^{(1)}, \beta^{(2)}, \dots, \beta^{(2p-1)})$, $\beta > 0$. satisfy*

$$\frac{j_p^{(m-2p+1, -\beta-m-1)} - 1}{2} \leq R_m(\Lambda_{2p}(\beta)) \leq \frac{j_p^{(m-p, -\beta-m-p)} - 1}{2},$$

where $j_p^{(\alpha, \beta)}$ refers to the smallest zero of the non-standard Jacobi polynomial polynomial $P_p^{(\alpha, \beta)}$.

The upper and lower bounds for $R_m(\Lambda_{2p}(\beta))$ established in Theorem 4.9 are presented in the table below for various values of p, m and for $\gamma = 0.5$ and 10. The

exact values of the corresponding optimal threshold factors are computed using the algorithm outlined in Section 2.5.

p	Lower Bound	$R_m(\Lambda_{2p})$	Upper Bound
2	1.0718	$R_5(\Lambda_4) = 1.2000$	1.4365
3	0.1501	$R_5(\Lambda_6) = 0.2222$	0.4878
2	1.8020	$R_7(\Lambda_4) = 2.0000$	2.1678
3	0.4878	$R_7(\Lambda_6) = 0.6667$	0.8392
2	2.1678	$R_8(\Lambda_4) = 2.4000$	2.5339
3	0.6626	$R_8(\Lambda_6) = 0.8594$	1.0169

Table 4.3: Bounds for $R_m(\Lambda_{2p}(\beta))$ with $\beta = 0.5$

As we showed in [36], if the zeros of $\pi_p^F(\cdot, R)$ are integers then the optimal threshold factor $R_m(\Lambda_{2p}) = R$, where m is the largest zero of $\pi_p^F(\cdot, R)$. In the following, we shall apply this result to Meixner polynomial of degree 2.

Theorem 4.10. *Let $0 \leq n < m$ be integer such that $(m + n - 1)^2 > 4mn$. Set*

$$\beta = \frac{4mn}{(m + n - 1)^2 - 4mn}.$$

Then

$$R_m(\Lambda_4(\beta)) = \frac{m + n - 1}{2(\beta + 1)}.$$

The associated optimal threshold polynomial is given by

$$\phi_m(\Lambda_{2p})(x) = \omega_1 \left(1 + \frac{x}{R_m(\Lambda_4(\beta))}\right)^n + \omega_2 \left(1 + \frac{x}{R_m(\Lambda_4(\beta))}\right)^m,$$

where

$$\omega_1 = \frac{m - \beta R_m(\Lambda_4(\beta))}{m - n} \quad \omega_2 = \frac{\beta R_m(\Lambda_4(\beta)) - n}{m - n}.$$

Proof. The Meixner polynomial of degree 2 is given by

$$M_2(t; \beta, R) = t^2 - ((2\beta + 2)R + 1)t + \beta(1 + \beta)R^2.$$

Taking

$$\beta = \frac{4mn}{(m+n-1)^2 - 4mn} \quad \text{and} \quad R = \frac{m+n-1}{2(\beta+1)},$$

one can readily show that

$$M_2(t; \beta, R) = (t - m)(t - n).$$

Thus the degree two Meixner polynomial has only non-negative integer zeros and thus the result follows from Theorem 4.3. □

CHAPTER 5

CHRISTOFFEL TRANSFORM AND HIGH-EFFICIENT ALGORITHMS FOR THE COMPUTATION OF OPTIMAL THRESHOLD FACTORS

The complexity of the algorithm for computing the optimal threshold factors introduced in Chapter 2 grows exponentially with the number of stages m and the order p . To compute these factors for large values of m and p , we study the spectral Christoffel transformations of the discrete measure μ_R^F . This leads to a highly efficient and stable algorithm for computing the optimal threshold factors with the particularity that its complexity depends only on the order p .

This chapter is organized as follows. Section 5.1 reviews structural properties of optimal threshold polynomials, providing their explicit characterization. Section 5.2 presents an efficient method for computing optimal threshold factors for arbitrary p -absolutely monotone sequence Λ_4 . Section 5.3 introduces the Christoffel transform, integral spectra, and spectral radii, forming the theoretical foundation of the efficient

algorithm for the computation of the optimal threshold factors and their associated polynomials.

5.1 Structural property of the Optimal Threshold Polynomial

Generalizing and adapting the techniques introduced in the work of Bernstein in [32] and Ait-Haddou in [36], we can prove the following.

Theorem 5.1. *Let $\Lambda_{2p} = (\lambda_0, \lambda_1, \dots, \lambda_{2p-1})$ be an absolutely positive sequence. For any positive integers m and p such that $m \geq 2p - 1$, The optimal threshold polynomial has the structure*

$$\Phi_m(\Lambda_{2p})(x) = \sum_{k=1}^{2p-1} \alpha_k \left(1 + \frac{x}{R_m(\Lambda_{2p})} \right)^{m_k}, \quad (5.1)$$

where $\alpha_k \geq 0$ for all k , with $\alpha_{2p-1} > 0$; and the sequence of integers $0 \leq m_1 < m_2 < \dots < m_{2p-1} \leq m$ satisfies

$$m_{2k} = m_{2k-1} + 1, \quad k = 1, 2, \dots, p-1, \quad \text{and} \quad m_{2p-1} = m. \quad (5.2)$$

In other words, in the representation (5.2), the integers $(m_1, \dots, m_{2p-2})$ appear as pairs of consecutive integers, while the largest exponent is equal to m .

So far, we have considered sequences Λ_{2p-1} with $2p$ elements so that we can take advantage of Gaussian quadratures. The following theorem provides the optimal threshold of sequences of Λ_{2p+1} with $2p + 2$ elements in terms of an associated sequence with

only $2p$ elements.

Theorem 5.2. *Given a sequence $\Lambda_{2p+1} = (\lambda_0, \lambda_1, \dots, \lambda_{2p})$ of positive real numbers and assume that sequence $\Lambda_{2p-1} = (\lambda_1, \dots, \lambda_{2p})$ is a p -absolutely monotonic sequence. Then, for any integer $m \geq 2p$, we have*

$$R_{m+1}(\Lambda_{2p+1}) = R_m(\Lambda_{2p}),$$

and

$$\Phi_{m+1}(\Lambda_{2p})(x) = \lambda_0 + \int_0^x \Phi_m(\Lambda_{2p-1})(\xi) d\xi. \quad (5.3)$$

Proof. We first note, from (5.3), that if the polynomial $\Phi_m(\Lambda_{2p-1})$ belongs to $\Pi_m(\Lambda_{2p})$ if and only if $\Phi_{m+1}(\Lambda_{2p+1})$ belongs $\Pi_m(\Lambda_{2p})$. Moreover, differentiating both sides of (5.3), we obtain

$$\Phi'_{m+1}(\Lambda_{2p})(x) = \Phi_m(\Lambda_{2p-1})(x).$$

Since $\Phi_{m+1}(\Lambda_{2p})$ is absolutely monotonic on $[-R_{m+1}(\Lambda_{2p+1}), 0]$, it follows that $\Phi'_{m+1}(\Lambda_{2p})$ is also absolutely monotonic over $[-R_{m+1}(\Lambda_{2p+1}), 0]$ and therefore, $(\Lambda_{2p-1}), 0]$ and therefore, $R_{m+1}(\Lambda_{2p+1}) \leq R_m(\Lambda_{2p})$. To prove that $R_{m+1}(\Lambda_{2p+1}) \geq R_m(\Lambda_{2p})$ we proceed as follows.

Since the optimal threshold factor $R_m(\Lambda_{2p})$ is the largest real number for which the measure μ_R^F admits a positive quadrature with integer nodes smaller than m , there exists non-negative numbers such that

$$\int (x-t)^{2p-1} d\mu_{R_m(\Lambda_{2p})}^F(t) = \sum_{k=1}^{2p-1} \alpha_i (x-m_i)^{2p-1}.$$

Therefore, there exist positive real numbers β_i such that

$$\int (x-t)^{2p} d\mu_{R_m(\Lambda_{2p})}^F(t) = \sum_{k=1}^{2p} \beta_i (x - (m_i + 1))^{2p} + \beta_0 x^{2p}.$$

Therefore, according to Remark (2.3), we have $R_{m+1}(\Lambda_{2p+1}) \geq R_m(\Lambda_{2p})$. This concludes the proof. $\square$

5.2 An Efficient computation of $R_m(\Lambda_4)$

Let $\Lambda_4 = (\lambda_0, \lambda_1, \lambda_2, \lambda_3)$ be a p -absolutely monotone sequence and $m \geq 3$ be an integer. Let $\bar{R}$ be the unique positive real number such that the largest zero of the orthogonal polynomial $\pi_2^F(t; R)$ is equal to m . The polynomial $\pi_2^F(t; \bar{R})$ has two simple real roots, denoted $r_1(R) < r_2(R) = m$. According to Theorem 5.1, the exponents of the optimal threshold polynomial are then given by

$$m_1 = \lfloor r_1(R) \rfloor, \quad m_2 = m_1 + 1, \quad m_3 = m.$$

Therefore, the optimal threshold factor $R_m(\Lambda_4)$ is the positive solution of the polynomial equation in R

$$\int (m_1 - t)(m_2 - t)(m - t) d\mu_R^F(t) = 0. \quad (5.4)$$

Example 5.1. Consider the sequence $\Lambda_4 = (1, 0.5, 0.5, 1)$. The associated orthogonal polynomial $\pi_2^F(t; R)$ has two strictly increasing real roots $r_1(R) < r_2(R)$ that tend to

infinity as $R \rightarrow \infty$. Therefore, the sequence Λ_4 is a p -absolutely monotone sequence.

We compute the optimal threshold factor $R_m(\Lambda_4)$ for various values of $m \geq 3$ by solving the polynomial equation in R

$$\int (m_1 - t)(m_2 - t)(m - t) d\mu_R^F(t) = 0, \quad (5.5)$$

where $m_1 = \lfloor r_1(R) \rfloor$ and $m_2 = m_1 + 1$.

The results are summarized in the table below.

m	$R_m(\Lambda_{2p})$	$r_1(R_m)$	m_1	m_2
10	3.7553	1.1929	1	2
100	38.4184	14.4013	14	15
1000	382.2370	145.7255	145	146
10000	3819.9360	1458.8094	1458	1459

Table 5.1: Optimal thresholds $R_m(\Lambda_4)$ associated with various m , for $\Lambda_4 = (1, 0.5, 0.5, 1)$.

5.3 Christoffel Transform and Spectral Properties

To generalize the idea of the efficient computation of the optimal threshold factor in the last section, we introduce the Christoffel transforms of the measure μ_R^F .

Definition 5.1 (Christoffel Transform). *For an admissible polynomial Ω , the Christoffel transform of μ_R^F is defined as*

$$\mu_R^{F,\Omega} := \Omega \mu_R^F = \sum_{j=0}^{\infty} \frac{\Omega(j) F^{(j)}(-R) R^j}{j!} \delta_j, \quad (5.6)$$

where the polynomial $\Omega(t)$ is called the annihilator polynomial of the measure $\mu_R^{F,\Omega}$.

If the measure μ_R^F is positive then clearly the Christoffel transform measure $\mu_R^{F,\Omega}$ is also positive. We shall denote by $\Pi_p^{R,\Omega}(t)$, $p \geq 1$, the associated orthogonal polynomials and their zeros are denoted by

$$\xi_{1,p}^\Omega < \xi_{2,p}^\Omega < \dots < \xi_{p,p}^\Omega.$$

Definition 5.2 (*p*-Configuration). *A sequence $\mathbf{n} = \{n_1, \dots, n_{p-1}\}$ with $1 \leq n_k \leq p - k + 1$ is called a *p*-configuration.*

We shall define several notions needed for the efficient algorithm. The techniques for the proof can be adapted from the work of Ait-Haddou [36] and will not be given here.

Definition 5.3 (Integral Spectrum). *For $\mathbf{n}$, $R > 0$, we define the integral spectrum $S(\mathbf{n}, R) = \{m_1, m_2, \dots, m_{2p-2}\}$ iteratively by*

$$m_1 = \lfloor \xi_{n_1,p}^{\Omega_0}(R) \rfloor, \quad m_2 = m_1 + 1, \quad \Omega_0 = \emptyset,$$

and for $k = 2, 3, \dots, p-1$,

$$m_{2k-1} = \lfloor \xi_{n_k,p-k+1}^{\Omega_{k-1}}(R) \rfloor, \quad m_{2k} = m_{2k-1} + 1, \quad \Omega_{k-1}(t) := \prod_{i=1}^{k-1} (m_{2i-1} - t)(m_{2i} - t).$$

The unique zero $\rho(\mathbf{n}, R)$ of the degree 1 polynomial orthogonal with respect to the measure $\mu_R^{F,\Omega_{p-1}}$ is called the spectral radius with respect to the couple $(\mathbf{n}, R)$. The

real number $\rho(\mathbf{n}, R)$ is given explicitly by

$$\rho(\mathbf{n}, R) = \frac{\int t P(t) d^F \mu_R(t)}{\int P(t) d\mu_R^F(t)} \quad \text{where} \quad P(t) = \prod_{j \in S(\mathbf{n}, R)} (t - j). \quad (5.7)$$

Given a positive integer m and a p -configuration $\mathbf{n}$, with $m \geq 2p - 1$, then, there exists a unique real number $\mathcal{R}_{m,p}(\mathbf{n})$ such that

$$\rho(\mathbf{n}, \mathcal{R}_{m,p}(\mathbf{n})) = m.$$

The real number $\mathcal{R}_{m,p}(\mathbf{n})$ will be called the *optimal spectral radius* with respect to the p -configuration $\mathbf{n}$ and the integer m . The associated integral spectrum

$$S(\mathbf{n}, \mathcal{R}_{m,p}(\mathbf{n})) = \{m_1, m_2, \dots, m_{2p-3}, m_{2p-2}\}$$

will be termed the *optimal integral spectrum* and denoted by $\mathcal{M}_{m,p}(\mathbf{n})$.

Proposition 5.1. *Let m and p be positive integers ($m \geq 2p - 1$) and $\mathbf{n}$ be a p -configuration. If R_1 and R_2 are two real numbers such that*

$$S(\mathbf{n}, R_1) = S(\mathbf{n}, R_2) \quad \text{and} \quad \rho(\mathbf{n}, R_1) \leq m \leq \rho(\mathbf{n}, R_2), \quad (5.8)$$

then the optimal integral spectrum with respect to $\mathbf{n}$ and to the integer m is given by $\mathcal{M}_{m,p}(\mathbf{n}) = S(\mathbf{n}, R_1) = S(\mathbf{n}, R_2)$ and the optimal spectral radius $\mathcal{R}_{m,p}(\mathbf{n})$ is the unique

positive real zero in $[R_1, R_2]$ of the polynomial equation in R

$$h_{2p-1}(m_1, m_2, \dots, m_{2p-2}, m; R) = 0, \quad (5.9)$$

where $(m_1, m_2, \dots, m_{2p-2}) = \mathcal{M}_{m,p}(\mathbf{n})$ and $h_{2p-1}(-, R)$ the polar form of the polynomial $\mathcal{H}_{2p-1}(\cdot; R)$.

The main theorem for efficient computation of optimal threshold factors, which can be proved using similar techniques as in Ait-Haddou [36] is the following.

Theorem 5.3. *Let m and p be positive integers such that $m \geq 2p - 1$. Let $\Lambda_{2p} = (\lambda_0, \lambda_1, \dots, \lambda_{2p-1})$ be an absolutely positive sequence and $\mathbf{n}$ be a p -configuration such that the system*

$$\int (x - t)^{2p-1} d\mu_{\mathcal{R}_{m,p}(\mathbf{n})} = \sum_{i=1}^{2p-1} \alpha_i (x - m_i)^{2p-1}, \quad (5.10)$$

where $(m_1, \dots, m_{2p-3}, m_{2p-2}) = \mathcal{M}_{m,p}(\mathbf{n})$ and $m_{2p-1} = m$, admits a non-negative solution in $(\alpha_1, \alpha_2, \dots, \alpha_{2p-1})$. Then

$$R_m(\Lambda_{2p} = \mathcal{R}_{m,p}(\mathbf{n})) \quad \text{and} \quad \Phi_m(\Lambda_{2p})(x) = \sum_{k=1}^{2p-1} \alpha_k \left(1 + \frac{x}{R_{m,2p-1}}\right)^{m_k}.$$

5.4 Computation of Christoffel Transformation for General Orthogonal Polynomials

In this section, we present a review of an algorithm for computing the orthogonal polynomials associated with the Christoffel transform of a measure, assuming the

three-term recurrence relation of its original orthogonal polynomials is known [39].

Let $\{P_n(t; R)\}_{n \geq 0}$ be a sequence of monic orthogonal polynomials satisfying

$$P_{n+1}(t; R) = (t - b_n)P_n(t; R) - g_n P_{n-1}(t; R), \quad P_{-1}(t; R) = 0, \quad P_0(t; R) = 1.$$

Then the orthogonal polynomials associated with the Christofel transform with innihilator polynomial Ω are given by

$$\Pi_p^\Omega(t; R) = \frac{1}{\Omega(t)} \begin{vmatrix} P_p(t; R) & P_{p+1}(t; R) & \dots & P_{p+2s}(t; R) \\ P_p(m_1; R) & P_{p+1}(m_1; R) & \dots & P_{p+2s}(m_1; R) \\ \vdots & \vdots & \ddots & \vdots \\ P_p(m_{2s}; R) & P_{p+1}(m_{2s}; R) & \dots & P_{p+2s}(m_{2s}; R) \end{vmatrix}. \quad (5.11)$$

where $\Pi_{-1}^\Omega(t) = 0$ and $\Pi_0^\Omega(t) = 1$. These orthogonal polynomials satisfy the three-term recurrence relation

$$\Pi_{n+1}^\Omega(t; R) = (t - B_n^{(2s)})\Pi_n^\Omega(t; R) - G_n^{(2s)}\Pi_{n-1}^\Omega(t; R), \quad n \geq 0,$$

where the coefficients B_n , G_n can be computed using the algorithm described below.

Algorithm 1 Christoffel Transformation for General Orthogonal Polynomials $(\Pi_p^\Omega)_{p \geq 1}$

1: **Input**

Parameters R, m, p

2: **Initialize** recurrence coefficients

$$B_j^{(0)} := b_j, \quad G_j^{(0)} := g_j, \quad j = 1, 2, \dots$$

3: **Apply Christoffel transformation iteratively for** $k = 1$ **to** $2s$

$$E_0 = 0, \quad Q_j = B_j^{(k-1)} - E_{j-1} - m_k, \quad E_j = \frac{G_{j+1}^{(k-1)}}{Q_j}$$

$$B_j^{(k)} = m_k + Q_j + E_j, \quad G_j^{(k)} = Q_j E_{j-1}$$

4: **Final recurrence coefficients**

$$B_j^{(2s)}, G_j^{(2s)}$$

5: **Output**

Integral spectrum $\{m_1, m_2, \dots, m_{2p-1}\}$

The roots of $\Pi_p^\Omega(t; R)$ are the eigenvalues of the tridiagonal matrix J_p

$$J_p = \begin{bmatrix} B_0^{(2s)} & \sqrt{G_1^{(2s)}} & & & \\ \sqrt{G_1^{(2s)}} & B_1^{(2s)} & \sqrt{G_2^{(2s)}} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{G_{p-1}^{(2s)}} & B_{p-1}^{(2s)} & \end{bmatrix}. \quad (5.12)$$

For instance, the three-term recurrence coefficient for Generalized Poisson–Charlier orthogonal polynomial with parameter $\gamma > 0$ are

$$b_j = \gamma R + j - 1, \quad g_j = (j - 1)\gamma R,$$

while for Meixner orthogonal polynomials with parameter $\beta > 0$ are

$$b_j = \frac{(1+c)j + \beta c}{1-c}, \quad g_j = \frac{cj(j + \beta - 1)}{(1-c)^2},$$

where $c = \frac{R}{1+R}$.

The following examples illustrate the computation of the integral spectrum for these two families of orthogonal polynomials using their spectral Chritoffel transform.

Example 5.2 (Generalized Poisson–Charlier). *Consider parameters $m = 100$, $p = 3$, $\gamma = 10$, and $R = 5$, with the configuration $n = \{1, 1\}$. Applying Algorithm 1 yields the following spectrum*

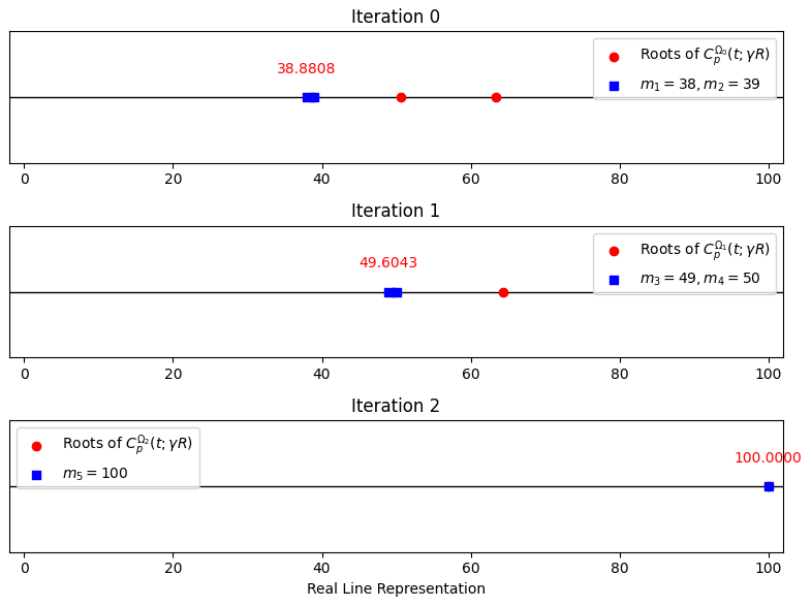


Figure 5.1: Spectrum associated with the Generalized Poisson–Charlier polynomials for $\gamma = 10, R = 5, p = 3, m = 100$.

Degree	Zeros of $C_p^\Omega(t; R)$	Selected Spectrum Values
3	{38.8808, 50.6686, 63.4505}	(38, 39)
2	{49.9788, 62.8696}	(49, 50)
Final Integral Spectrum		(38, 39, 49, 50, 100)

Table 5.2: Integral spectrum constructed from generalized Poisson–Charlier polynomials with parameters $\gamma = 10$, $R = 5$, $p = 3$, and $m = 100$.

Example 5.3 (Meixner). *Consider the Meixner case with $\beta = 3$, $R = 5$, $p = 3$, and $m = 100$. Algorithm 1 applied to the Meixner, the recurrence coefficients results in the spectrum shown below.*

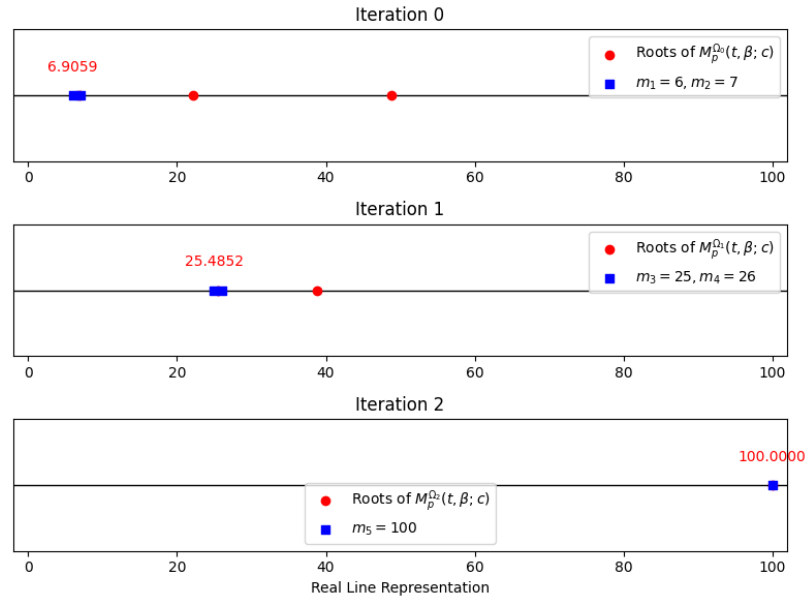


Figure 5.2: Spectrum associated with Meixner polynomials for $\beta = 3$, $R = 5$, $p = 3$, $m = 100$.

Degree	Zeros of $M_p^\Omega(t, \beta; R)$	Selected Spectrum Values
3	{ 6.9059, 22.2219, 48.8723 }	(6, 7)
2	{25.4852, 38.7892 }	(25, 26)
Final Integral Spectrum		(6, 7, 25, 26, 100)

Table 5.3: Integral spectrum constructed from Meixner polynomials with parameters $\beta = 3$, $R = 5$, $p = 3$, and $m = 100$.

The algorithm presented computes the optimal threshold factor $R_m(\Lambda_{2p})$ and the corresponding optimal polynomial (5.1).

The algorithm and the obtained results are illustrated below for the case of generalized Poisson-Charlier sequences.

Algorithm 2 Computing $R_m(\Lambda_{2p})$ and $\Phi_m(\Lambda_{2p})(x)$

Require: Positive integer m ($m \geq 2p - 1$), polynomial degree p , scaling parameter

$\gamma > 0$

- 1: Initialize $R_{\max} = \ell_p^{(m-p)}/\gamma$, $R_{\min} = \ell_p^{(m-2p+1)}/\gamma$
- 2: Set $\alpha_k = -1$, $k = 1, 2, \dots, 2p - 1$
- 3: **while** one of the $\alpha_k < 0$, $k = 1, 2, \dots, 2p - 1$ **do**
- 4: Select randomly a p -configuration n
- 5: Compute $R_{\max}$, $R_{\min}$, and R_{mid}
- 6: Compute spectrum $S_{m,p}(n)$

$$S_{m,p}(n) = \{m_1, m_2, \dots, m_{2p-2}\}$$

- 7: Compute α_k , $k = 1, 2, \dots, 2p - 1$

$$\alpha_k = \sum_{i=1}^p w_i \prod_{\substack{j=1 \\ j \neq k}}^{2p} \frac{m_j - \xi_i}{m_j - m_k}$$

- 8: **end while**
- 9: Set $R_m(\Lambda_{2p}) = R_{m,p}$, $S_m(\Lambda_{2p}) = S_{m,p}(n) \cup \{m\}$
- 10: Compute $\Phi_m(\Lambda_{2p})(x)$

$$\Phi_m(\Lambda_{2p})(x) = \sum_{k=1}^{2p-1} \alpha_k \left(1 + \frac{x}{R_{m,p}}\right)^{m_k}$$

return $R_m(\Lambda_{2p})$, $S_m(\Lambda_{2p})$, a_k , $k = 1, 2, \dots, 2p - 1$, $\Phi_m(\Lambda_{2p})(x)$

m	$R_m(\Lambda_{2p})$	$S_m(\Lambda_{2p})$	α_k
15	0.865	(4, 5, 6, 7, 15)	(0.049, 0.388, 0.458, 0.102, 0.003)
25	1.669	(10, 11, 13, 14, 25)	(0.033, 0.342, 0.493, 0.129, 0.004)
35	2.510	(17, 18, 20, 21, 35)	(0.027, 0.319, 0.506, 0.143, 0.005)
45	3.373	(24, 25, 28, 29, 45)	(0.024, 0.305, 0.513, 0.153, 0.005)
55	4.250	(32, 33, 36, 37, 55)	(0.022, 0.296, 0.517, 0.159, 0.006)
65	5.138	(40, 41, 44, 45, 65)	(0.021, 0.289, 0.520, 0.164, 0.006)
75	6.035	(48, 49, 53, 54, 75)	(0.020, 0.284, 0.522, 0.168, 0.007)
85	6.938	(56, 57, 61, 62, 85)	(0.019, 0.279, 0.523, 0.172, 0.007)
95	7.846	(64, 65, 70, 71, 95)	(0.018, 0.276, 0.524, 0.175, 0.007)
105	8.759	(72, 73, 78, 79, 105)	(0.018, 0.273, 0.525, 0.177, 0.007)
115	9.677	(80, 81, 87, 88, 115)	(0.017, 0.270, 0.526, 0.179, 0.007)
125	10.598	(89, 90, 96, 97, 125)	(0.017, 0.268, 0.527, 0.181, 0.007)
135	11.522	(97, 98, 104, 105, 135)	(0.017, 0.266, 0.527, 0.182, 0.008)
145	12.449	(106, 107, 113, 114, 145)	(0.017, 0.264, 0.528, 0.184, 0.008)
155	13.378	(114, 115, 122, 123, 155)	(0.016, 0.263, 0.528, 0.185, 0.008)
165	14.309	(123, 124, 131, 132, 165)	(0.016, 0.261, 0.528, 0.186, 0.008)
175	15.243	(132, 133, 140, 141, 175)	(0.016, 0.260, 0.529, 0.187, 0.008)
185	16.178	(140, 141, 149, 150, 185)	(0.016, 0.259, 0.529, 0.188, 0.008)
195	17.115	(149, 150, 158, 159, 195)	(0.016, 0.258, 0.529, 0.189, 0.008)

Table 5.4: Optimal spectral radius, spectrum, and α_k w.r.t Generalized Poisson-Charlier Measure; $p = 3, \gamma = 10$ for different m values.

CHAPTER 6

POSITIVITY PRESERVING EXPONENTIAL INTEGRATORS

In this chapter, we begin by reviewing exponential integrator methods, followed by a discussion of the necessary and sufficient conditions for these schemes to preserve positivity. Building on the results from the preceding sections, we derive explicit formulas for low-order optimal positivity-preserving exponential integrators. Particular emphasis is placed on optimal schemes whose collocation points coincide with the zeros of classical orthogonal polynomials.

This chapter is organized as follows.

Section 6.1 reviews Metzler matrices and their structure-preserving properties, with a focus on positivity preservation. Section 6.2 reviews exponential integrators and derives accuracy conditions. Sections 6.3, 6.4 and 6.5 investigate optimal schemes with specific collocation points (zeros of orthogonal polynomials and related polynomials) and provide explicit low-order expressions.

6.1 Metzler Matrices and Structure-Preserving Properties

In this section, we review and analyze Metzler matrices, focusing particularly on their role in positivity preservation. We highlight fundamental results connecting Metzler matrices to non-negative matrix exponentials and explore their implications in contractivity and dissipativity analysis.

6.1.1 Metzler Matrices and Positivity Preservation

Definition 6.1. [53] *Given a real matrix $A = (a_{ij}) \in \mathbb{R}^{s \times s}$, we say that A is Metzler if it satisfies*

$$a_{ij} \geq 0 \quad \text{for all } i \neq j.$$

These matrices naturally arise in various applications, particularly in the study of dynamical systems and control design [53], [54]. Metzler matrices are also associated with *contractivity* and *dissipative structures* in numerical methods and stability analysis. In this section, we explore these properties in detail and demonstrate their importance in preserving structure in both continuous and discrete settings.

The characterization of matrices A for which exponential matrix e^{tA} has non-negative entries for any $t \geq 0$ plays a fundamental role in this chapter.

Proposition 6.1. [55] *Let A be a square matrix. The matrix $e^{tA} \geq 0$ for all $t \geq 0$ if and only if A is a Metzler.*

Proof. Assume that $e^{tA} \geq 0$ for all $t \geq 0$. Expanding the matrix exponential as

$$e^{tA} = I + tA + O(t^2).$$

we conclude that there exists $t_0 > 0$ such that $I + t_0A \geq 0$, and therefore

$$t_0 a_{ij} \geq 0 \quad \text{for all } i \neq j.$$

Since $t_0 \geq 0$, we conclude that $a_{ij} \geq 0$ for all $i \neq j$, that is A is a Metzler matrix.

Conversely, assume that A is Metzler. Then there exists $\rho > 0$ such that $A + \rho I \geq 0$

and therefore, $e^{(A+\rho I)t} \geq 0$ for any $t \geq 0$. Moreover, $e^{(-\rho I)t} \geq 0$ for any $t \geq 0$ and

since $-\rho I$ and $A + \rho I$ commute, we have $0 \leq e^{(A+\rho I)t} e^{(-\rho I)t} = e^{tA}$. This concludes the

proof. $\square$

Consider the following initial-value problem

$$\frac{du}{dt} = Au(t) + f(t), \quad u(0) = u_0, \quad u_0 \in \mathbb{R}^s, \quad (6.1)$$

where A is a square matrix of order s and $f : \mathbb{R} \longrightarrow \mathbb{R}^s$.

Theorem 6.1. [14] *Let A be a Metzler matrix. If $u_0 \geq 0$ and $f(t) \geq 0$ for all $t \geq 0$, then the solution to (6.1) satisfies $u(t) \geq 0$ for all $t \geq 0$.*

Proof. The solution to the initial-value problem (6.1) is given by

$$u(t) = e^{At}u_0 + \int_0^t e^{(t-\tau)A}f(\tau) d\tau. \quad (6.2)$$

Since A is Metzler, by Proposition 6.1, $e^{tA} \geq 0$ for all t . Therefore, we readily conclude from (6.2), that $u(t) \geq 0$ for all $t \geq 0$, completing the proof. $\square$

Theorem 6.2. [14] *Let $A \in \mathbb{R}^{s \times s}$. If the solution to (6.1) satisfies $u(t) \geq 0$ for all $t \geq 0$ whenever $u_0 \geq 0$ and $f(t) \geq 0$, then A is a Metzler matrix.*

Proof. We prove the theorem by contradiction. Suppose that A is not a Metzler matrix. Then, according to Proposition 6.1, there exists $t_0 \geq 0$ such that at least one entry $b_{i_0 j_0}(t)$ of the matrix $e^{tA} = (b_{ij})$ negative for any $0 < t \leq t_0$. Consider first the case where $f = 0$. The solution simplifies to $u(t) = e^{tA}u_0$. Choosing

$$u_0 = [0, 0, \dots, 1_{j_0}, 0, \dots, 0]^T,$$

it follows that the $u(t_0) = e^{t_0 A}u_0$ has a negative entry, leading to a contradiction. Consider now the case $f \neq 0$. Taking $u_0 = [0, 0, \dots, 0]^T$ and f as

$$f(t) = [0, 0, \dots, 0, 1, 0, \dots, 0]^T,$$

and applying (6.2), we obtain

$$u(t_0) = \int_0^{t_0} e^{(t_0 - \tau)A} f(\tau) d\tau$$

and which has at least a negative entry. This concludes the proof. $\square$

6.1.2 Contractivity and Dissipativity

Consider the initial value problem arising from the discretization of the second-order spatial derivative using central differences.

$$\frac{du}{dt} = -Au + f, \quad u(0) = 0, \quad f \geq 0, \quad (6.3)$$

where A is a non-singular matrix.

Definition 6.2. [15] *The initial-value problem (6.3), with A a non-singular matrix, is said to be non-negatively posed if the solution satisfies*

$$0 \leq u(t) \leq -A^{-1}f \quad \text{for all } t \geq 0$$

and for all constant forcing $f \geq 0$ and $u_0 = 0$.

Definition 6.3. [56] *A non-singular matrix B is called an M -matrix if $(-B)$ is Metzler and $B^{-1} \geq 0$.*

Theorem 6.3. [15] *The initial-value problem (6.3) is non-negatively posed if and only if the matrix $-A$ is an M -matrix.*

Proof. If the matrix $-A$ is an M -matrix then A is Metzler and therefore, according to Theorem 6.1, $u(t) \geq 0$ for any $f \geq 0$. In the case the forcing term is constant and $u_0 = 0$, from (6.2), the solution of the initial-value problem is given by

$$u(t) = (-I - e^{tA})A^{-1}f.$$

Therefore

$$-A^{-1}f - u(t) = -A^{-1}f - (e^{tA} - I)A^{-1}f = e^{tA}A^{-1}f.$$

Therefore, if $-A$ is an M-matrix, we have $e^{tA} \geq 0$ and $A^{-1} \leq 0$. Therefore, $u(t) \leq -A^{-1}f$ for any $f \geq 0$. $\square$

6.2 Exponential Integrators

In this section, we revisit exponential integrator methods as applied to initial-value problems. Furthermore, we emphasize the significance of the optimal threshold factors in the design of exponential integrators that guarantee positivity preservation.

Consider the initial-value problem (1.1). Using the variation of the constants method, the solution to (1.1) is given by

$$u(t) = e^{At}u_0 + \int_0^t e^{(t-\tau)A}f(\tau)d\tau. \quad (6.4)$$

It is shown in [14] that a necessary and sufficient condition for (1.1) to preserve positivity for all non-negative functions f , i.e.; if $u_0 \geq 0$ then $u(t) \geq 0$ for $t \geq 0$, is that A is a Metzler matrix, i.e.; all the off-diagonal elements of A are non-negative.

From (6.4), we have

$$u(t_{n+1}) = e^{hA}u(t_n) + \int_0^h e^{(h-\tau)A}f(t_n + \tau)d\tau,$$

where $t_n = nh$, ($h > 0$). A change of variable leads to

$$u(t_{n+1}) = e^{hA}u(t_n) + \int_0^1 e^{h(1-\theta)A}f(t_n + h\theta)d\theta. \quad (6.5)$$

A numerical scheme for solving (1.1) can be obtained by approximating the function f within the integral by its interpolating polynomial in certain non-confluent nodes $c_1, c_2, \dots, c_p$, i.e.; replacing $f(t_n + h\theta)$ inside the integral (6.5) by

$$\sum_{k=1}^p \ell_k(\theta)f(t_n + c_k\theta),$$

where $\ell_k, k = 1, 2, \dots, p$, are the basic Lagrange polynomials

$$\ell_k(\theta) = \prod_{m=1, m \neq k}^p \frac{\theta - c_m}{c_k - c_m}.$$

This leads to the scheme

$$u_{n+1} = e^{hA}u_n + h \sum_{i=1}^p b_i(hA)f(t_n + c_ih), \quad (6.6)$$

where

$$b_i(hA) = \int_0^1 e^{h(1-\theta)A} \ell_i(\theta) d\theta.$$

Denote by φ_k the entire functions

$$\varphi_k(z) = \int_0^1 e^{(1-\theta)z} \frac{\theta^{k-1}}{(k-1)!} d\theta, \quad k \geq 1. \quad (6.7)$$

We have

$$\varphi_k(z) = \frac{1}{k!} + \frac{z}{(k+1)!} + \frac{z^2}{(k+2)!} + \dots + \frac{z^n}{(k+n)!} + \dots$$

The functions $b_k(z)$ can be written as linear combination of the functions $\varphi_k(z)$ as

$$b_k(z) = \frac{1}{\prod_{m=1, m \neq k}^p (c_k - c_m)} \sum_{j=1}^p (-1)^{p-j} (j-1)! \sigma_{p-j}(\hat{c}_k) \varphi_j(z). \quad (6.8)$$

where $\hat{c}_k$ refers to $(c_1, \dots, c_{k-1}, c_{k+1}, \dots, c_p)$ and σ_ℓ refer to the elementary symmetric functions. Thus, the scheme (6.6) can be written in terms of the functions $\varphi_k, k = 1, 2, \dots, p$.

Example For $p = 1$, the scheme (6.6) is given by

$$u_{n+1} = e^{hA} u_n + h \varphi_1(hA) f(t_n + c_1 h).$$

The choice $c_1 = 0$ leads to the exponential Euler quadrature method, while the choice $c_1 = 1/2$ yields the exponential midpoint rule.

Example For $p = 2$, the scheme (6.6) is given by

$$u_{n+1} = e^{hA} u_n + h [b_1(hA) f(t_n + c_1 h) + b_2(hA) f(t_n + c_2 h)],$$

where

$$\begin{aligned} b_1(z) &= \frac{c_2}{c_2 - c_1} \varphi_1(z) - \frac{1}{c_2 - c_1} \varphi_2(z), \\ b_2(z) &= -\frac{c_1}{c_2 - c_1} \varphi_1(z) + \frac{1}{c_2 - c_1} \varphi_2(z). \end{aligned}$$

The choice $c_1 = 0$ and $c_2 = 1$ yields the exponential trapezoid rule with expansions of b_1 and b_2 as

$$b_1(z) = \sum_{k=0}^{\infty} \frac{k+1}{(k+2)!} z^k, \quad b_2(z) = \sum_{k=0}^{\infty} \frac{1}{(k+2)!} z^k,$$

Example For $p = 3$, the scheme (6.6) is given by

$$u_{n+1} = e^{hA} u_n + h [b_1(hA)f(t_n + c_1 h) + b_2(hA)f(t_n + c_2 h) + b_3(hA)f(t_n + c_3 h)],$$

where

$$\begin{aligned} b_1(z) &= \frac{1}{(c_1 - c_2)(c_1 - c_3)} [c_2 c_3 \varphi_1(z) - (c_2 + c_3) \varphi_2(z) + 2 \varphi_3(z)], \\ b_2(z) &= \frac{1}{(c_2 - c_1)(c_2 - c_3)} [c_1 c_3 \varphi_1(z) - (c_1 + c_3) \varphi_2(z) + 2 \varphi_3(z)], \\ b_3(z) &= \frac{1}{(c_3 - c_1)(c_3 - c_2)} [c_1 c_2 \varphi_1(z) - (c_1 + c_2) \varphi_2(z) + 2 \varphi_3(z)]. \end{aligned}$$

It is shown in [12] that if $f^{(p)} \in L^1([0, T])$, $T > 0$, then the scheme obtained in (6.6) have order of convergence p , more precisely, the error bound

$$\|u(t_n) - u_n\| \leq Ch^p \int_0^T \|f^{(p)}(\tau)\| d\tau \quad (6.9)$$

holds uniformly on $0 \leq t_n \leq T$, with a constant that depends on T , but is independent on the step-size h . The norm $\|\cdot\|$ in Equation (6.9) represents any norm defined on the space $\mathbb{R}^s$.

In practice, the exponential function and the analytic functions b_i , $i = 1, 2, \dots, p$, in scheme (6.6) are approximated by rational functions. To maintain the desired order

of convergence, these rational functions must satisfy specific conditions, which will be outlined subsequently. Consider the schemes

$$u_{n+1} = r_0(hA)u_n + h \sum_{i=1}^p r_i(hA)f(t_n + c_i h), \quad (6.10)$$

where $r_0, r_1, \dots, r_p$ are rational functions. Following [14], we define

Definition 6.4. *The scheme (6.10) is said to be accurate for order s if*

$$u(t_{n+1}) - r_0(hA)u(t_n) + h \sum_{i=1}^p r_i(hA)f(t_n + c_i h) = O(h^{s+1}) \quad \text{as } h \longrightarrow 0,$$

for any choice of the matrix A and smooth function f .

The following is proven in [14].

Theorem 6.4. *The scheme (6.10) is of order s if and only if*

$$r_0(z) - e^z = O(z^{s+1}) \quad \text{as } z \longrightarrow 0, \quad (6.11)$$

and for $\ell = 0, 1, \dots, s-1$,

$$\frac{\ell!}{z^{\ell+1}} \left(r_0(z) - \sum_{j=0}^{\ell} \frac{z^j}{j!} \right) - \sum_{j=1}^p c_j^{\ell} r_j(z) = O(z^{s-\ell}) \quad \text{as } z \longrightarrow 0. \quad (6.12)$$

Definition 6.5. *The scheme (6.10) is said to preserve positivity if for any $u_0 \geq 0$ and non-negative function f , we have $u_n \geq 0$ for $n \geq 0$.*

Clearly the scheme (6.10) preserves positivity if and only if

$$r_i(hA) \geq 0 \quad \text{for } i = 0, 1, \dots, s.$$

To ensure positivity preservation, we impose an additional condition on the functions $r_i(x)$. If each $r_i(x)$ is *absolutely monotonic* over $[-R, 0]$, then positivity follows. The following is shown in [14].

Theorem 6.5. [14] *Given a Metzler matrix A and assume that all the rational functions $r_i, i = 0, 1, \dots, p$, are absolutely monotonic over the interval $[-r, 0]$. Then the scheme (6.10) preserves positivity for any step size h satisfying*

$$h \leq \frac{r}{\sigma(A)} \quad \text{where } \sigma(A) = \max_{a_{ii} < 0} |a_{ii}|. \quad (6.13)$$

Proof. Since A is Metzler, we have

$$A + \sigma I \geq 0 \quad \text{where } \sigma := \sigma(A) = \max_{a_{ii} < 0} |a_{ii}|.$$

Writing $r_k(hA)$ as $r_k(hA + h\sigma I - h\sigma I)$ and Expanding $r_k(hA)$ around $A + \sigma I$ using Taylor expansion, we obtain

$$r_k(hA) = \sum_{m=0}^N \frac{r_k^{(m)}(-h\sigma)h^m}{m!} (A + \sigma I)^m.$$

Since r_k is absolutely monotonic on $[-r, 0]$, h satisfies (6.13) and the matrix $A + \sigma I$

is non-negative, it follows that

$$r_k^{(m)}(-h\sigma) \geq 0, \quad \text{for all } m \geq 0.$$

Therefore, $r_k(hA) \geq 0$ for $k = 0, 1, \dots, p$. Therefore, the scheme (6.10) with $u_0 \geq 0$ and $f(t) \geq 0$ preserves nonnegativity, i.e.;

$$u_{n+1} = r_0(hA)u_n + h \sum_{j=1}^p r_j(hA)f(t_n + c_j h) \geq 0.$$

This concludes the proof. □

Theorem 6.6. *Let R be a positive real number and r be a polynomial such that $r(hA) \geq 0$ for any Metzler matrix A of any order and such that $h\sigma(A) \leq R$. Then r is absolutely monotonic on $[-R, 0]$.*

Proof. Let N be the degree of the polynomial r . Consider the Metzler matrix A of order $N + 1$ with diagonal values $-R/h$ and subdiagonal values $\epsilon > 0$. The matrix A can be decomposed as

$$A = \epsilon B - \frac{R}{h}I,$$

where B is a matrix with diagonal values 0 and subdiagonal values equal to 1, i.e.;

$$B = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 1 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 & 0 \end{bmatrix}.$$

Applying the Taylor series expansion around $-RI$, we obtain

$$r(hA) = \sum_{m=0}^N \frac{r_k^{(m)}(-R)h^m}{m!} \epsilon^m B^m.$$

Since $r(hA) \geq 0$ for any $\epsilon > 0$ and the element of $r(hA)$ at the $(k+1)^{em}$ row and the first column is given by

$$(r(hA))_{k+1,1} = \frac{r^{(k)}(-R)h^k \epsilon^k B^k}{k!} + O(\epsilon^{k+1}) \quad \text{as } \epsilon \rightarrow 0$$

Thus, $r^{(k)}(-R) \geq 0$ for any k . Therefore, r is absolutely monotonic over $[-R, 0]$. this concludes the proof. $\square$

The previous two theorem can be re-stated that given α , the quantity

$$H = \frac{\min\{R(r_0), R(r_1), \dots, R(r_p)\}}{\alpha}, \quad (6.14)$$

is the greatest $H \in [0, \infty]$ the scheme (6.10) preserve positivity for all stepsizes $h \in (0, H)$ and all positivity preserving matrices A with diagonal elements larger than $-\alpha$.

In this work, we shall restrict ourselves to the case where the rational functions $r_i, i = 0, 1, \dots, p$, are polynomials and study the following family of schemes.

$$u_{n+1} = Q_0(hA)u_n + h \sum_{i=1}^p Q_i(hA)f(t_n + c_i h), \quad (6.15)$$

where $Q_0, Q_1, \dots, Q_p$, are polynomials of degree $m \geq p$ such that

$$Q_0(z) - e^z = O(z^{p+1}) \quad \text{as } z \longrightarrow 0, \quad (6.16)$$

and for $i = 1, 2, \dots, p$,

$$Q_i(z) - b_i(z) = O(z^p) \quad \text{as } z \longrightarrow 0. \quad (6.17)$$

We have the following result regarding the order of these methods.

Theorem 6.7. *The schemes (6.15) with condition (6.16) and (6.17) are of order p .*

Proof. We need to check that our polynomials $Q_j, j = 0, \dots, p$, satisfy the conditions given in Theorem 6.4. The condition (6.11) is satisfied by definition of the schemes.

For (6.12), we proceed as follows.

For $\ell = 0, 1, \dots, p-1$, we have

$$\sum_{j=1}^p c_j^\ell Q_j(z) = \sum_{j=1}^p c_j^\ell b_j(z) + O(z^p) = \ell! \varphi_{\ell+1}(z) - O(z^p),$$

and

$$\frac{\ell!}{z^{\ell+1}} \left(Q_0(z) - \sum_{j=0}^{\ell} \frac{z^j}{j!} \right) = \ell! \varphi_{\ell+1}(z) + O(z^{p-\ell}).$$

This shows that (6.12) holds and concludes the proof.

□

Example First order schemes of the form (6.15) are given by

$$u_{n+1} = Q_0(hA)u_n + hQ_1(hA)f(t_n + c_1h).$$

where Q_0 and Q_1 are of the form $Q_0(x) = 1 + x + \sum_{k=2}^m a_k x^k$ and $Q_1(x) = 1 + \sum_{k=1}^m b_k x^k$, where $a_2, \dots, a_m$ and $b_1, \dots, b_m$ are arbitrary real numbers. Thus the polynomial $Q_0 \in \Pi_m(\Lambda_2)$ and $Q_1 \in \Pi_m(\Lambda_1)$ where $\Lambda_2 = (1, 1)$ and $\Lambda_1 = (1)$.

Example Second order schemes of the form (6.15) are given by

$$u_{n+1} = Q_0(hA)u_n + h[Q_1(hA)f(t_n + c_1h) + Q_2(hA)f(t_n + c_2h)] \quad (6.18)$$

where Q_0, Q_1 and Q_2 are of the form

$$Q_0(x) = 1 + x + \frac{x^2}{2!} + \sum_{k=3}^m a_k x^k, \quad Q_i(x) = \lambda_0^{(i)} + \lambda_1^{(i)}x + \sum_{k=2}^m d_k^{(i)}x^k, \quad i = 1, 2$$

where

$$\lambda_0^{(1)} = \frac{2c_2 - 1}{2(c_2 - c_1)}, \quad \lambda_1^{(1)} = \frac{3c_2 - 1}{6(c_2 - c_1)}, \quad \lambda_0^{(2)} = \frac{1 - 2c_1}{2(c_2 - c_1)}, \quad \lambda_1^{(2)} = \frac{1 - 3c_1}{6(c_2 - c_1)}.$$

Thus $Q_0 \in \Pi_m[(1, 1, 1)]$, $Q_i \in \Pi_m[(\lambda_0^{(i)}, \lambda_1^{(i)})]$, $i = 1, 2$.

Theorem 6.8. *There is no one-step numerical method of order greater than 1 that preserves positivity unconditionally.*

Proof. Consider the general scheme (6.10). Suppose that the method preserves positivity unconditionally, meaning that $u_n \geq 0$ and $f(t) \geq 0$ imply $u_{n+1} \geq 0$ for all $h > 0$.

This requires that each $r_k(z)$ is absolutely monotonic on $(-\infty, 0]$

Now assume the method has order at least 2. Then consistency with the exact solution $u(t_{n+1}) = e^{hA}u_n + \dots$ implies that

$$r_0(z) = e^z + O(z^3) \quad \text{as } z \rightarrow 0.$$

Applying the Bolley–Crouzeix Lemma ?? to r_0 , we conclude

$$r_0(z) = e^z \quad \text{for all } z \in (-\infty, 0].$$

But this is impossible, because r_0 is a rational function (as required by the one-step structure), while e^z is not a rational function.

Hence, there is no choice of rational functions r_k that are absolutely monotonic and satisfy the order condition $r_0(z) = e^z + O(z^3)$. This contradiction proves the claim. □

6.3 Exponential Integrators with Collocation Points as Zeros of Orthogonal Polynomials and Re- lated Polynomials

It is a challenging problem to characterize collocation points $c_i, i = 1, 2, \dots, p$, for which all the coefficients in (6.20) are positive. The positivity of these coefficients is paramount as it ensures the existence of step-sizes for which the corresponding

schemes preserve positivity. In this section, we provide a general expression of the polynomial $Q_j, j = 0, 1, \dots, p$, of the schemes (6.15) of order p . In particular, we show the positivity of (6.20) when the collocation points are the zeros of Legendre polynomials or the zeros of a linear combination of Legendre polynomials and their derivatives.

We recall that for $\alpha, \beta > -1$, the Jacobi polynomials $J_n^{(\alpha, \beta)}, n \geq 0$, are defined as the orthogonal polynomials with respect to the weight $(1-t)^\alpha t^\beta$, i.e.;

$$\int_0^1 J_n^{(\alpha, \beta)}(t) J_m^{(\alpha, \beta)}(t) (1-t)^\alpha t^\beta dt = h_{nm} \delta_{nm}.$$

Legendre polynomials are defined by $J_n^{(0,0)}$ Chebyshev polynomials of the first and second kind T_n and S_n are defined respectively by

$$T_n(t) = P_n^{(-\frac{1}{2}, -\frac{1}{2})}(t), \quad S_n(t) = P_n^{(\frac{1}{2}, \frac{1}{2})}(t).$$

The Gegenbauer (or ultra-spherical) polynomials C_n^μ are defined by

$$C_n^\mu(t) = P_n^{(\mu-\frac{1}{2}, \mu-\frac{1}{2})}(t).$$

From the analytic expansion of the function φ_k given in (6.7) and formula (6.8), the polynomials Q_j are of the form

$$Q_0(x) = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \dots + \frac{x^p}{p!} + a_{p+1}x^{p+1} + \dots + a_mx^m,$$

where $a_{p+1}, \dots, a_m$ are arbitrary real numbers, and for $k = 1, \dots, p$,

$$Q_k(z) = \sum_{\ell=0}^{p-1} \frac{\lambda_\ell^{(k)}}{\ell!} z^\ell + \sum_{\ell=p}^m d_\ell^{(k)} z^\ell,$$

where $d_\ell^{(k)}, \ell = p, \dots, m$ and $k = 1, 2, \dots, p$ are arbitrary real numbers and

$$\lambda_\ell^{(k)} = \frac{1}{(\ell+1) \prod_{m=1, m \neq k}^p (c_k - c_m)} \sum_{j=1}^p (-1)^{p-j} \frac{\sigma_{p-j}(\hat{c}_k)}{\binom{j+\ell}{j-1}}.$$

A compact expression of the coefficients $\lambda_\ell^{(k)}$ can be achieved using the polar form of the polynomials

$$G_{\ell,p}(x) = \frac{1}{(\ell+1) \binom{p+\ell}{p-1}} \sum_{j=0}^{p-1} (-1)^j \binom{p+\ell}{j} x^j. \quad (6.19)$$

More precisely, we have

$$\lambda_\ell^{(k)} = \frac{g_{\ell,p}(c_1, c_2, \dots, c_{k-1}, c_{k+1}, \dots, c_p)}{\prod_{m=1, m \neq k}^p (c_k - c_m)}, \quad \ell = 0, 1, \dots, p-1, \quad (6.20)$$

where $g_{\ell,p}$ is the polar form of the polynomial $G_{\ell,p}$. Summarizing

Proposition 6.2. *The polynomials $Q_j, j = 0, 1, \dots, p$, of the schemes (6.15) of order p satisfy*

$$Q_0 \in \Pi_m(\Lambda_{p+1}^{(0)}), \quad Q_j \in \Pi_m(\Lambda_p^{(j)}), \quad j = 1, 2, \dots, p, \quad (6.21)$$

where

$$\Lambda_{p+1}^{(0)} = (1, 1, \dots, 1), \quad \Lambda_p^{(j)} = (\lambda_0^{(j)}, \dots, \lambda_{p-1}^{(j)}),$$

where the coefficients $\lambda_\ell^{(j)}, j = 0, 1, \dots, p$ and $\ell = 0, 1, \dots, p-1$, are given by (6.20).

Remark 6.1. From the expression (6.20), the polynomials $G_{\ell,p}$, $0 \leq \ell \leq p-1$, can be written as

$$G_{\ell,p}(x) = \sum_{j=1}^p \lambda_{\ell}^{(j)} (c_j - x)^{p-1}. \quad (6.22)$$

Identifying the two polynomials leads to the following identities between the coefficients $\lambda_{\ell}^{(k)}$ and the collocation points $c_1, c_2, \dots, c_p$

$$\sum_{k=1}^p \lambda_{\ell}^{(k)} c_k^j = \frac{\binom{p+\ell}{p-j-1}}{(\ell+1)\binom{p+\ell}{p-1}}, \quad j = 0, 1, \dots, p; \quad \ell = 0, 1, \dots, p-1.$$

In the following, we will derive an integral representation for the polynomials $G_{\ell,p}$, which will enable the computation of the coefficients $\lambda_k^{(\ell)}$ for specific collocation points $c_1, c_2, \dots, c_p$.

Theorem 6.9. The polynomials $G_{\ell,p}$ in (6.19) are given by

$$G_{\ell,p}(x) = \int_0^1 (1-t)^{\ell} (t-x)^{p-1} dt, \quad \ell = 0, 1, \dots, p-1.$$

Proof. We have

$$\begin{aligned} \int_0^1 (1-t)^{\ell} (t-x)^{p-1} dt &= \sum_{j=0}^{p-1} (-1)^j \binom{p-1}{j} x^j \int_0^1 (1-t)^{\ell} t^{p-1-j} dt \\ &= \sum_{j=0}^{p-1} (-1)^j \binom{p-1}{j} x^j \frac{\ell!(p-1-j)!}{(p+\ell-j-1)!} = \sum_{j=0}^{p-1} (-1)^j x^j \frac{\ell!(p-1)!}{(p+\ell-j)!} \\ &= \frac{\ell!(p-1)!}{p+\ell)!} \sum_{j=0}^{p-1} (-1)^j x^j \binom{p+\ell}{j} = G_{\ell,p}(x). \end{aligned}$$

This concludes the proof.

□

Corollary 6.1. *When the collocation points, $c_1, c_2, \dots, c_p$, are the zeros of the Legendre polynomial $J_p^{(0,0)}$ over the interval $[0, 1]$, the coefficients $\lambda_\ell^{(k)}$ are positive and given by*

$$\lambda_\ell^{(k)} = (1 - c_k)^\ell \omega_k, \quad \ell = 0, 1, \dots, p-1; \quad k = 1, 2, \dots, p,$$

where $\omega_1, \omega_2, \dots, \omega_p$ are the weight of the Gaussian quadrature with respect to the Lebesgue measure dt .

Proof. According to Gauss quadrature, we have

$$G_{\ell,p}(x) = \int_0^1 (1-t)^\ell (t-x)^{p-1} dt = \sum_{k=1}^p (1-c_k)^\ell \omega_k (c_k-x)^{p-1}.$$

Comparing with (6.22) concludes the proof.

□

We can take advantage of the fact that the polynomials $G_{\ell,p}$ are of degree only $p-1$, while we are searching quadratures with p nodes. Let $c_1, c_2, \dots, c_p$ be the zeros of the polynomial

$$P(t) = J_p^{(0,0)}(t) + \alpha \frac{d}{dt} J_p^{(0,0)}(t), \quad \alpha \in \mathbb{R}. \quad (6.23)$$

It is well-known that we have a $(2p-2, p)$ -quadrature with positive weights and node the zeros of P , that is

$$\int_0^1 f(t) dt = \sum_{k=1}^p \mu_k f(c_k), \quad (6.24)$$

for any polynomial f of degree $2p-2$. Thus, a similar proof as of Corollary 6.1

provides the following.

Proposition 6.3. *If the collocation points $c_1, c_2, \dots, c_p$ are the zeros of the polynomial P in (6.23), then the coefficients $\lambda_k^{(\ell)}$ in (6.20) are positive and are given by*

$$\lambda_k^{(\ell)} = (1 - c_k)^\ell \mu_k, \quad \ell = 0, 1, \dots, p-1; \quad k = 1, 2, \dots, p,$$

where $\mu_1, \mu_2, \dots, \mu_p$ are the weights of the $(2p-2, p)$ quadrature given in (6.24).

In general and using Gaussian quadrature, we have the following.

Corollary 6.2. *The coefficients $\lambda_\ell^{(k)}$ are given by*

$$\lambda_\ell^{(k)} = \frac{1}{S'(c_k)} \int_0^1 (1-t)^\ell \frac{S(t)}{t-c_k} dt = \sum_{i=1}^p \omega_i (1-\xi_i)^\ell \frac{S(\xi_i)}{(\xi_i - c_k) S'(c_k)},$$

where $S(t) = (t - c_1)(t - c_2) \dots (t - c_p)$ and ξ_i, ω_i are the nodes and weights of the Gaussian quadrature with respect to dt .

We remark that for the collocation points of Corollary 6.1 and Proposition 6.3, the sequences $(\lambda_0^{(k)}, \lambda_1^{(k)}, \dots, \lambda_{p-1}^{(k)})$ are generalized Poisson-Charlier sequences for any $1 \leq k \leq p$. Consequently, the results established in the preceding chapters can be employed to compute their optimal threshold factors.

It is natural to ask if there are collocation points for which the associated sequences are Meixner sequence for any $0 \leq k \leq p$. The following theorem provide a negative answer to the question.

Theorem 6.10. *There do not exist collocation points $c_k \in (0, 1), k = 1, \dots, p$, such that the associated sequences $(\lambda_0^{(k)}, \lambda_1^{(k)}, \dots, \lambda_{p-1}^{(k)})$ are Meixner sequences for any $1 \leq$*

$k \leq p$, i.e.;

$$\lambda_\ell^{(k)} = (\beta_k)^\ell, \quad \beta_k > 0,$$

and satisfy the integral identity

$$\int_0^1 (1-t)^\ell (t-x)^{p-1} dt = \sum_{k=1}^p \alpha_\ell^{(k)} (c_k - x)^{p-1} \quad (6.25)$$

for all $\ell = 0, 1, \dots, p-1$.

Proof. Setting $x = 0$ in (6.25) and take successively $\ell = 1$ and $\ell = 2$, we obtain

$$\int_0^1 (1-t) t^{p-1} dt = \sum_{k=1}^p \beta_k c_k^{p-1}, \quad (6.26)$$

$$\int_0^1 (1-t)^2 t^{p-1} dt = \sum_{k=1}^p \beta_k (\beta_k + 1) c_k^{p-1}. \quad (6.27)$$

Subtracting (6.26) from (6.27), we get

$$-\int_0^1 t^p (1-t) dt = \sum_{k=1}^p \beta_k^2 c_k^{p-1}.$$

The left side is strictly negative, whereas the right side is strictly positive. This contradiction concludes the proof. $\square$

6.4 Optimal Exponential Quadrature Integrators

The schemes (6.15) are such that

$$Q_0 \in \Pi_m(\Lambda_{p+1}^{(0)}), \quad Q_j \in \Pi_m(\Lambda_p^{(j)}), \quad j = 1, 2, \dots, p, \quad (6.28)$$

where

$$\Lambda_{p+1}^{(0)} = (1, 1, \dots, 1), \quad \Lambda_p^{(j)} = (\lambda_0^{(j)}, \dots, \lambda_{p-1}^{(j)}),$$

where the coefficients $\lambda_\ell^{(j)}$ $j = 0, 1, \dots, p$ and $\ell = 0, 1, \dots, p$ are given by (6.20).

Theorem 6.5 provides restrictions on the step-size for the schemes to preserve positivity. Therefore, to obtain efficient exponential integrators, we should choose positivity preserving schemes with the largest possible step-size. This prompts the following definition

Definition 6.6. *Optimal exponential integrator schemes of order p and stage m associated with the collocation points $(c_1, c_2, \dots, c_p)$ are defined by*

$$u_{n+1} = \Phi_m \left(\Lambda_{p+1}^{(0)} \right) (hA) u_n + h \sum_{j=1}^p \Phi_m \left(\Lambda_p^{(j)} \right) (hA) f(t_n + c_j h), \quad (6.29)$$

where $\Phi_m(\Lambda^j)$, $j = 0, 1, \dots, p$ are the optimal threshold polynomial associated with the sequence $\Lambda_p^{(j)}$. The optimal threshold factor of the scheme (6.29) is defined by

$$R_{m,p} = \min \left(R_m \left(\Lambda_{p+1}^{(0)} \right), R_m \left(\Lambda_p^{(1)} \right), \dots, R_m \left(\Lambda_p^{(p)} \right) \right).$$

Thus according to Theorem 6.5, the optimal scheme (6.29) preserves positivity for

any step-size h such that

$$h \leq \frac{R_{m,p}}{\sigma(A)} \quad \text{where} \quad \sigma(A) = \max_{a_{ii} < 0} |a_{ii}|.$$

Example 6.1. *In the following we shall use the algorithm described in Section 5, to give the optimal scheme of order 4 and stage $m = 5$, for the collocation points*

$$(c_1, c_2, c_3, c_4) = \left(\frac{1}{15}, \frac{3}{10}, \frac{3}{5}, \frac{9}{10} \right).$$

We have the sequence $\Lambda_5^{(0)} = (1, 1, 1, 1, 1)$. To compute the other sequences we use formula (6.20). This gives

$$\begin{aligned} \Lambda_4^{(1)} &= (0.1639, 0.1543, 0.1430, 0.1336), & \Lambda_4^{(2)} &= (0.2804, 0.1931, 0.1376, 0.0960), \\ \Lambda_4^{(3)} &= (0.3171, 0.1296, 0.0498, 0.0202), & \Lambda_4^{(4)} &= (0.2385, 0.0230, 0.0030, 0.0002). \end{aligned}$$

Using the algorithm of Section 5, we find

$$\begin{aligned} R_5(\Lambda_5^{(0)}) &= 2, & R_5(\Lambda_4^{(1)}) &= 2.7897, & R_5(\Lambda_4^{(2)}) &= 3.9416, \\ R_5(\Lambda_4^{(3)}) &= 5.9891, & R_5(\Lambda_4^{(4)}) &= 16.4674. \end{aligned}$$

Therefore, the optimal threshold factor of the scheme is $R_{5,4} = 2$. The associated

optimal polynomials are given by

$$\begin{aligned}
\Phi_5(\Lambda_5^{(0)}) &= 0.2 + 0.666 \left(1 + \frac{x}{2}\right)^2 + 0.1333 \left(1 + \frac{x}{2}\right)^5, \\
\Phi_5(\Lambda_4^{(1)}) &= 0.0424 \left(1 + \frac{x}{2.7897}\right) + 0.073 \left(1 + \frac{x}{2.7897}\right)^2 + 0.0483 \left(1 + \frac{x}{2.7897}\right)^5, \\
\Phi_5(\Lambda_4^{(2)}) &= 0.0935 \left(1 + \frac{x}{3.9416}\right) + 0.0555 \left(1 + \frac{x}{3.9416}\right)^2 + 0.0979 \left(1 + \frac{x}{3.9416}\right)^5, \\
\Phi_5(\Lambda_4^{(3)}) &= 0.0745 \left(1 + \frac{x}{5.9891}\right) + 0.1703 \left(1 + \frac{x}{5.9891}\right)^2 + 0.07222 \left(1 + \frac{x}{5.9891}\right)^5, \\
\Phi_5(\Lambda_4^{(4)}) &= 0.1164 + 0.1103 \left(1 + \frac{x}{16.4674}\right)^3 + 0.01118 \left(1 + \frac{x}{16.4674}\right)^4.
\end{aligned}$$

The table below provides the optimal threshold factors of schemes of the form (6.15) with collocation points the zeros of Jacobi polynomials $J_n^{(\alpha, \beta)}$ for different values of the parameters α and β . For instance, when the collocation points are the zeros of Chebyshev polynomials T_3 , we have $R_{5,3} = 0$. This means that at least one of the coefficients $\lambda_\ell^{(k)}$ in (6.20) is negative and thus there is no scheme of the form (6.15) with $m = 5$ and collocation points the zeros of T_3 for which positivity preservation is guaranteed.

(α, β)	$R_{4,3}$	$R_{5,3}$	$R_{6,4}$	$R_{7,4}$	$R_{8,4}$	$R_{8,5}$
$(0, 0)$	2	2.6506	2.6506	3.5184	4.2879	3.3733
$(-\frac{1}{2}, -\frac{1}{2})$	0	0	2.6506	3.5184	4.2879	0
$(1, 0)$	2	2.6506	2.6506	3.3535	3.5634	2.8418
$(0, 1)$	0	0	0	0	0	0
$(\frac{1}{2}, \frac{1}{2})$	2	2.6506	0	0	0	0

Table 6.1: Values of the optimal threshold factors of several sequences Λ_3 as computed with our algorithm.

6.5 Optimal Schemes of Low Orders

In this section, we provide explicit expressions of the optimal exponential integrators of first, second and third orders.

Theorem 6.11. *The optimal first order scheme associated with a single collocation point c_1 is given by*

$$u_{n+1} = \left(I + \frac{h}{m} A \right)^m u_n + hf(t_n + c_1 h).$$

The optimal threshold factor of the scheme is $R_{m,1} = m$.

Proof. We have the sequence $\Lambda_2^{(0)} = (1, 1)$ and $\Lambda_1^{(1)} = (1)$. According to Proposition 2.2, we have

$$\Phi_m(\Lambda_2^{(0)}) = \left(1 + \frac{x}{m} \right)^m.$$

This concludes the proof. □

Theorem 6.12. *The optimal scheme of order 2 associated with collocation points (c_1, c_2) such that*

$$c_1 < \frac{1}{3} \quad \text{and} \quad c_2 > \frac{1}{2}, \tag{6.30}$$

is given by

$$\begin{aligned} u_{n+1} = & \left[\frac{I}{m} + \frac{m-1}{m} \left(I + \frac{hA}{m-1} \right)^m \right] u_n \\ & + h \frac{2c_2 - 1}{2(c_2 - c_1)} \left(I + \frac{(3c_2 - 1)hA}{3m(2c_2 - 1)} \right)^m f(t_n + c_1 h) \\ & + h \frac{1 - 2c_2}{2(c_2 - c_1)} \left(I + \frac{(1 - 3c_1)hA}{3m(1 - 2c_1)} \right)^m f(t_n + c_2 h). \end{aligned}$$

The optimal threshold factor is given by

$$R_{m,2} = \min \left(m - 1, \frac{3m(2c_2 - 1)}{3c_2 - 1}, \frac{3m(1 - 2c_1)}{1 - 3c_1} \right).$$

Proof. According to (6.20), we have $\Lambda_3^{(0)} = (1, 1, 1)$ and

$$\Lambda_2^{(1)} = \left(\frac{2c_2 - 1}{2(c_2 - c_1)}, \frac{3c_2 - 1}{6(c_2 - c_1)} \right), \quad \Lambda_2^{(2)} = \left(\frac{1 - 2c_1}{2(c_2 - c_1)}, \frac{1 - 3c_1}{6(c_2 - c_1)} \right).$$

According to Propositions 2.2 and 2.3, we have

$$\Phi_m(\Lambda_3^{(0)}) = \frac{1}{m} + \frac{m-1}{m} \left(1 + \frac{x}{m-1} \right)^m, \quad R_m(\Lambda_2^{(0)}) = m - 1,$$

and

$$\begin{aligned} \Phi_m(\Lambda_2^{(1)}) &= \frac{2c_2 - 1}{2(c_2 - c_1)} \left(1 + \frac{(3c_2 - 1)x}{3(2c_2 - 1)} \right)^m, & R_m(\Lambda_2^{(1)}) &= \frac{3m(2c_2 - 1)}{3c_2 - 1}, \\ \Phi_m(\Lambda_2^{(2)}) &= \frac{1 - 2c_1}{2(c_2 - c_1)} \left(1 + \frac{(1 - 3c_1)x}{3(1 - 2c_1)} \right)^m, & R_m(\Lambda_2^{(2)}) &= \frac{3m(1 - 2c_1)}{1 - 3c_1}. \end{aligned}$$

This concludes the proof. □

For collocation points (c_1, c_2) that does not satisfy the condition (6.30), the optimal threshold factor $R_{m,2} = 0$, i.e.; no guarantee that the schemes preserve positivity.

We shall give explicit expressions for optimal schemes of order 3 when m is a square. The main reason is that it is shown in [36], [33] that if m is a square, then

$R_m([1, 1, 1, 1]) = m - \sqrt{m}$ and

$$\Phi_m([1, 1, 1, 1])(x) = \frac{\sqrt{m}}{2\sqrt{m}-1} \left(1 + \frac{x}{m-\sqrt{m}}\right)^{m-2\sqrt{m}+1} + \frac{\sqrt{m}-1}{2\sqrt{m}-1} \left(1 + \frac{x}{m-\sqrt{m}}\right)^m.$$

Thus, using this result and Proposition 2.3 and the coefficients expressed in (6.20),

we obtain the following.

Theorem 6.13. *If m is a square, then the optimal positivity preserving scheme of order 3 and stage m associated with the collocation points (c_1, c_2, c_3) is given by*

$$u_{n+1} = \left[\frac{\sqrt{m}}{2\sqrt{m}-1} \left(I + \frac{hA}{m-\sqrt{m}} \right)^{m-2\sqrt{m}+1} + \frac{\sqrt{m}-1}{2\sqrt{m}-1} \left(I + \frac{hA}{m-\sqrt{m}} \right)^m \right] u_n \\ + \sum_{i=1}^3 h \left[\left(\lambda_0^{(i)} - \frac{(m-1)(\lambda_1^{(i)})^2}{m\lambda_2^{(i)}} \right) I + \frac{(m-1)(\lambda_1^{(i)})^2}{m\lambda_2} \left(I + \frac{\lambda_2^{(i)}hA}{(m-1)\lambda_1^{(1)}} \right)^m f(t_n + c_i h) \right],$$

where for $i = 1, 2, 3$,

$$\lambda_0^{(i)} = \frac{2 + 6c_2c_3 - 3(c_2 + c_3)}{6 \prod_{j=1, j \neq i}^3 (c_i - c_j)}, \quad \lambda_1^{(i)} = \frac{1 + 6c_2c_3 - 2(c_2 + c_3)}{12 \prod_{j=1, j \neq i}^3 (c_i - c_j)}, \quad \lambda_2^{(i)} = \frac{2 + 20c_2c_3 - 5(c_2 + c_3)}{120 \prod_{j=1, j \neq i}^3 (c_i - c_j)},$$

provides that $\lambda_k^{(\ell)} > 0$ for $k = 0, 1, 2$ and $\ell = 1, 2, 3$ and

$$\lambda_0^{(i)} \geq \frac{(\lambda_1^{(i)})^2(m-1)}{\lambda_2^{(i)}m} \quad \text{for } i = 1, 2, 3.$$

The optimal threshold factor is given by

$$\min \left(m - \sqrt{m}, \frac{(m-1)\lambda_1^{(1)}}{\lambda_2^{(1)}}, \frac{(m-1)\lambda_1^{(2)}}{\lambda_2^{(2)}}, \frac{(m-1)\lambda_1^{(3)}}{\lambda_2^{(3)}} \right).$$

CHAPTER 7

APPLICATION OF POSITIVITY-PRESERVING EXPONENTIAL INTEGRATOR SCHEMES TO SEMI-DISCRETIZED PARTIAL DIFFERENTIAL EQUATIONS

This chapter applies the positivity-preserving exponential integrator schemes developed in the previous chapters to time-dependent partial differential equations after spatial discretization. The focus is on demonstrating how optimal exponential schemes ensure numerical stability, maintain non-negativity, and control oscillations under appropriate step-size constraints. A variety of numerical experiments confirm the theoretical threshold factors and validate the preservation of qualitative properties such as positivity and contractivity.

In section 7.1, we test the exponential integrators schemes to a transport equation and investigates how step size and polynomial degree influence stability and positivity. In Section 7.2, we simulate a solar thermal storage model governed by a heat equation with a time-varying Gaussian source, illustrating the scheme's robustness and the

impact of exceeding positivity thresholds. Finally, Section 7.3 explores transient heat conduction with internal generation, reinforcing the necessity of step-size restrictions for stable, physically meaningful results.

7.1 Numerical Experiments

Consider the initial-boundary value problem

$$\begin{cases} \frac{\partial}{\partial t} V(x, t) = -\frac{\partial}{\partial x} V(x, t) + F(x, t) & (t \geq 0) \\ V(0, t) = 0 & (t \geq 0) \\ V(x, 0) = v_0(x) & (0 \leq x \leq 1), \end{cases}$$

where v_0 is a given initial condition. We assume that $F(x, t) \geq 0$ in $[0, 1] \times [0, \infty)$ and that $v_0(x) \geq 0$ in $[0, 1]$. We fix $s \geq 1$ and write $\Delta x = 1/s$ and $x_j = j\Delta x, j = 0, 1, \dots, s$. We define $U(t) = (U_0(t), U_1(t), \dots, U_s(t)), f(t) = (f_0(t), f_1(t), \dots, f_s(t))$ and $\tilde{U} = (\tilde{U}_0, \tilde{U}_1, \dots, \tilde{U}_s)$ by

$$U_j(t) := V(x_j, t), \quad f_j(t) = F(x_j, t), \quad \tilde{U}_j = v_0(x_j), \quad j = 0, 1, \dots, s.$$

Approximating the space derivative by the first backward difference method with mesh size Δx as

$$\frac{\partial}{\partial x} V(x_j, t) \simeq (\Delta x)^{-1} (V(x_j, t) - V(x_{j-1}, t)), \quad j = 1, 2, \dots, s,$$

we obtain the initial-value problem

$$\frac{d}{dt}U(t) = AU(t) + f(t), \quad U(0) = \tilde{U}, \quad (7.1)$$

with

$$A = (\Delta x)^{-1} \begin{pmatrix} -1 & & & & \\ 1 & -1 & & & \\ & 1 & -1 & & \\ & & \ddots & \ddots & \\ & & & 1 & -1 \end{pmatrix}.$$

Since the matrix A is Metzler and the vector f has positive components for any $t \geq 0$, the solution to (7.1) is positive. According to Theorem 6.5, the optimal schemes (6.29) applied to the initial-boundary value problem (7.1) is guaranteed to preserve positivity if

$$\frac{h}{\Delta x} \leq R_{m,p}. \quad (7.2)$$

The ability to maintain positivity in the solution, even with larger time steps h relative to spatial steps Δx , is a key practical advantage of choosing optimal schemes for solving (7.1). In our numerical tests, we have chosen $s = 250$, $U(0) = (1, 0, 0, \dots, 0)^T$ and $f_j(t) = (0, 1, 0, 0, \dots, 0)^T$ for any $t > 0$ and we integrated until $t = 0.4$. Given a vector $y = (y_1, y_2, \dots, y_s)$, we shall denote by $\sigma(y)$ the number of sign changes within the sequence $(y_1, y_2, \dots, y_s)$ where zero values are disregarded.

Our numerical simulations, detailed in Tables 7.1 and 7.2, confirm that when condition (7.2) is met, the optimal schemes preserve positivity, indicated by $\sigma(u_n) = 0$.

$m = 5, p = 3, R_{m,p} = 2.6506$	
$h/\Delta x$	$\sigma(u_n)$
4	1347
3	1027
2.7	365
2.6	0
2	0
1	0
$m = 7, p = 3, R_{m,p} = 4.2879$	
$h/\Delta x$	$\sigma(u_n)$
6	886
5	1182
4.3	136
4.1	0
3	0
2	0

$m = 6, p = 3, R_{m,p} = 3.5184$	
$h/\Delta x$	$\sigma(u_n)$
4	1772
3.7	1608
3.5	0
3	0
2	0
1	0

Table 7.1: Optimal schemes with Legendre collocation points.

$m = 4, p = 3, R_{m,p} = 2$	
$h/\Delta x$	$\sigma(u_n)$
4	1065
3	1615
2.5	1976
2	0
1.5	0
1	0
$m = 8, p = 5, R_{m,p} = 2.8418$	
$h/\Delta x$	$\sigma(u_n)$
4	2239
3	0
2.9	0
2.8	0
2.5	0
2	0

$m = 7, p = 4, R_{m,p} = 3.3535$	
$h/\Delta x$	$\sigma(u_n)$
4	1764
3.7	1376
3.6	670
3.5	0
3	0
2.5	0

Table 7.2: Optimal schemes with collocation points the zeros of Jacobi polynomials $J_p^{(1,0)}(t)$.

In Table 7.2, with $m = 8$ and $p = 5$, we observe $\sigma(u_n) = 0$ for $h/\Delta x = 3$ and 4, despite condition (7.2) not being met. However, this does not guarantee positivity in all scenarios, i.e.; we can construct a Metzler matrix A and positive vectors $U(0)$ and

$f(t)$ where $\sigma(u_n) > 0$.

In the following, we select the parameter $s = 100$. The first table corresponds to the second optimal scheme with the initial condition $U_0 = (0, 2, 0, 0, \dots, 0)$, while the forcing term is defined as $F(x, t) = (1, 0, \dots, 0)$. The remaining three tables use the initial function $v_0(x) = \cos(x + \pi) + 1$ and the forcing function $F(x, t) = (\sin(2t) + 1)(\cos(5x) + 1)$.

For all cases, integration is performed until $t = 2$. Let N be the number of integration steps and m the polynomial degree; the total number of matrix-vector multiplications is then $F = Nm$. To maintain consistency in comparison across methods, we keep F constant for each row in the table.

To evaluate the numerical solution u , we compute $\sigma(u)$, which counts the number of sign changes, and also report the minimum value $\min(u)$. The numerical results are analyzed by varying the step size h and the polynomial degree m while keeping the initial condition and forcing term unchanged.

7.1.1 Second-Order Optimal Scheme Validation

For the second-order scheme, we analyzed different step sizes with a fixed $\Delta x = 0.01$ and an optimal threshold factor $R_m(\Lambda_2) = m - 1$.

The results, summarized in Table 7.3, confirm that positivity requirement when the step size ratio $h/\Delta x \leq R_m(\Lambda_2)$. Exceeding this threshold might lead to negative solution or even instability of the solution. Specifically, positivity is lost at $h/\Delta x = 6.30$ for $m = 5$, and at $h/\Delta x = 9.00$ for $m = 7$. For $m = 10$, stability persists until

N	F	$h/\Delta x$	$ u_N _\infty$	$\sigma(u_N)$	$\min(u)$
$(m = 5) \quad \phi = \phi_5(\Lambda_2)$					
21	105	9.20	3.82×10^{55}	97	-3.77×10^{55}
22	110	9.00	8.15×10^{56}	97	-8.15×10^{56}
31	155	6.30	4.63×10^{45}	70	-4.63×10^{45}
33	165	6.00	6.42×10^{38}	67	-6.42×10^{38}
47	235	4.20	3.74×10^0	57	-3.74
50	250	4.00	1.41×10^{-2}	0	0.01
66	330	3.00	1.26×10^{-2}	0	0.01
$(m = 7) \quad \phi = \phi_7(\Lambda_2)$					
21	147	9.20	1.40×10^{43}	78	-1.40×10^{43}
22	154	9.00	5.57×10^{41}	75	-3.03×10^{41}
31	217	6.30	7.18×10^{-1}	39	-0.63
33	231	6.00	1.49×10^{-2}	0	0.00
47	329	4.20	1.32×10^{-2}	0	0.01
50	350	4.00	1.29×10^{-2}	0	0.01
66	462	3.00	1.21×10^{-2}	0	0.01
$(m = 10) \quad \phi = \phi_{10}(\Lambda_2)$					
21	210	9.20	2.04×10^{-2}	14	-0.01
22	220	9.00	1.54×10^{-2}	0	0.00
31	310	6.30	1.42×10^{-2}	0	0.00
33	330	6.00	1.40×10^{-2}	0	0.00
47	470	4.20	1.26×10^{-2}	0	0.01
50	500	4.00	1.24×10^{-2}	0	0.01
66	660	3.00	1.18×10^{-2}	0	0.01

Table 7.3: Numerical results for different m values, second-order optimal scheme

$h/\Delta x = 9.20$, beyond which minor oscillations appear.

7.1.2 Numerical Testing with Legendre Collocation Points

For numerical testing with Legendre collocation points and fixed $\Delta x = 0.01$, the results confirm that stability and positivity are preserved within the theoretical thresholds of $h/\Delta x \leq R_{m,p}$. Table 7.5 shows that for $m = 5$, stability holds up to $h/\Delta x = 2.99$, but instability emerges at $h/\Delta x = 3.52$. Similarly, for $m = 7$, numerical solutions remain

stable up to the threshold of $h/\Delta x = 3.52$, beyond which instability sets in.

The 2D colormap and 3D solution plots further illustrate the transition from stable propagation to severe instability as the step size increases beyond the positivity limit. These results emphasize adhering to the derived step size constraints to ensure numerical reliability.

N	F	$h/\Delta x$	$ u_N _\infty$	$\sigma(u_N)$	$\min(u)$
$(m = 5) \quad \phi = \phi_5(\Lambda_3)$					
51	255	3.87	2.646475×10^{18}	2811	-2.646475×10^{18}
56	280	3.52	2.215654×10^9	2774	-9.141546×10^8
66	330	2.99	1.459987×10^0	0	0.000000×10^0
90	450	2.20	1.462155×10^0	0	0.000000×10^0
100	500	2.00	1.465517×10^0	0	0.000000×10^0
200	1000	1.00	1.466545×10^0	0	0.000000×10^0
$(m = 5) \quad \phi = \phi_5(\Lambda_4)$					
51	255	3.87	7.953217×10^{47}	3012	-7.953217×10^{47}
56	280	3.52	7.458928×10^{40}	3383	-3.701290×10^{40}
66	330	2.99	2.783403×10^{27}	4031	-1.746838×10^{27}
90	450	2.20	2.725659×10^0	1	-4.713026×10^{-2}
100	500	2.00	1.466050×10^0	0	0.000000×10^0
200	1000	1.00	1.467583×10^0	0	0.000000×10^0
$(m = 7) \quad \phi = \phi_7(\Lambda_4)$					
51	357	3.87	4.002987×10^0	38	-2.076908×10^0
66	462	2.99	1.460445×10^0	0	0.000000×10^0
90	630	2.20	1.462896×10^0	0	0.000000×10^0
100	700	2.00	1.466332×10^0	0	0.000000×10^0
200	1400	1.00	1.468168×10^0	0	0.000000×10^0

Table 7.4: Numerical results for different m values, $\Phi_m(\Lambda_p)$ with p Legendre collocation points

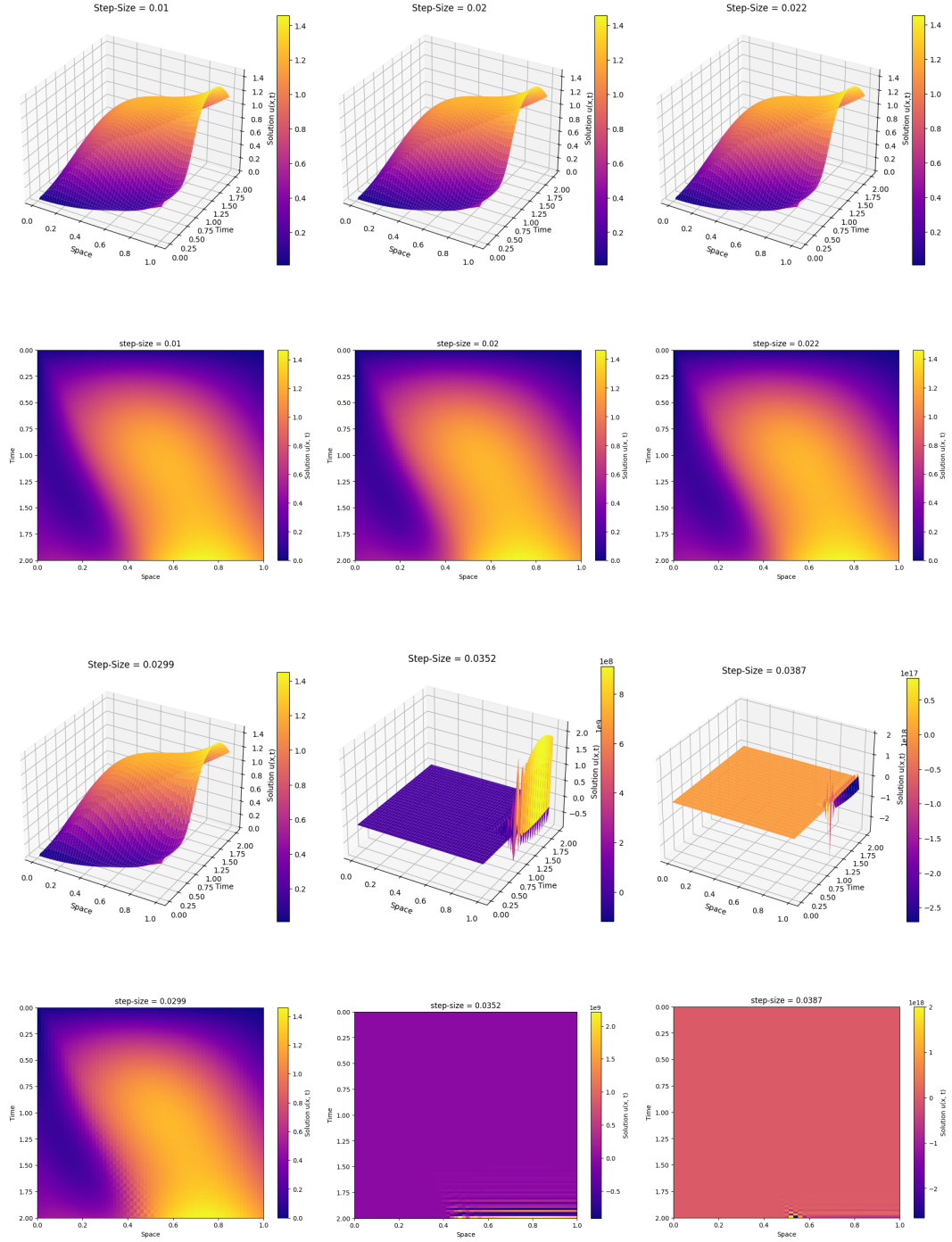


Figure 7.1: Comparison of numerical solutions for $m = 5, \phi_5(\Lambda_3), R_5(\Lambda_3) = 2.65$

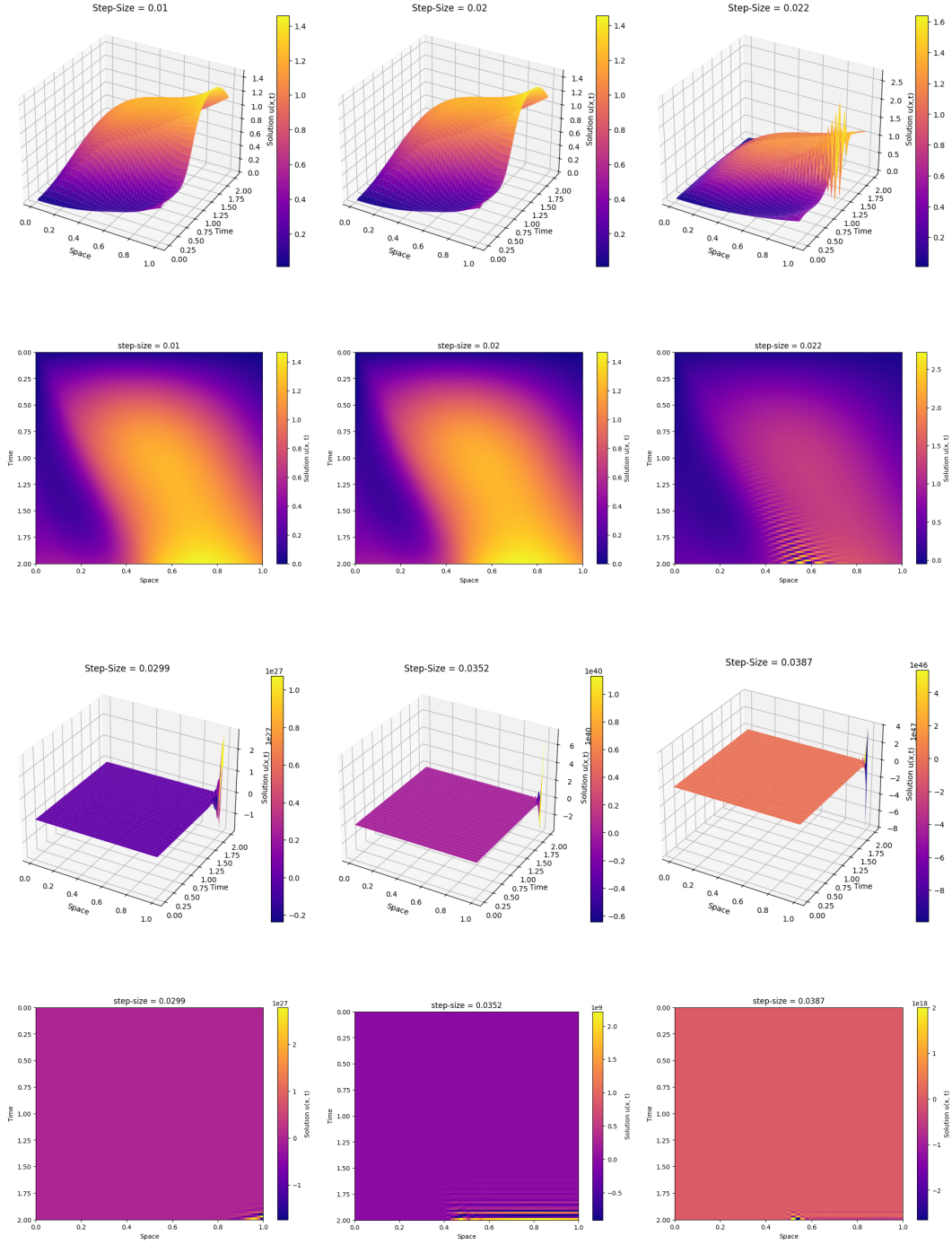


Figure 7.2: Comparison of numerical solutions for $m = 5$, $\phi_5(\Lambda_4)$, $R_5(\Lambda_4) = 2$

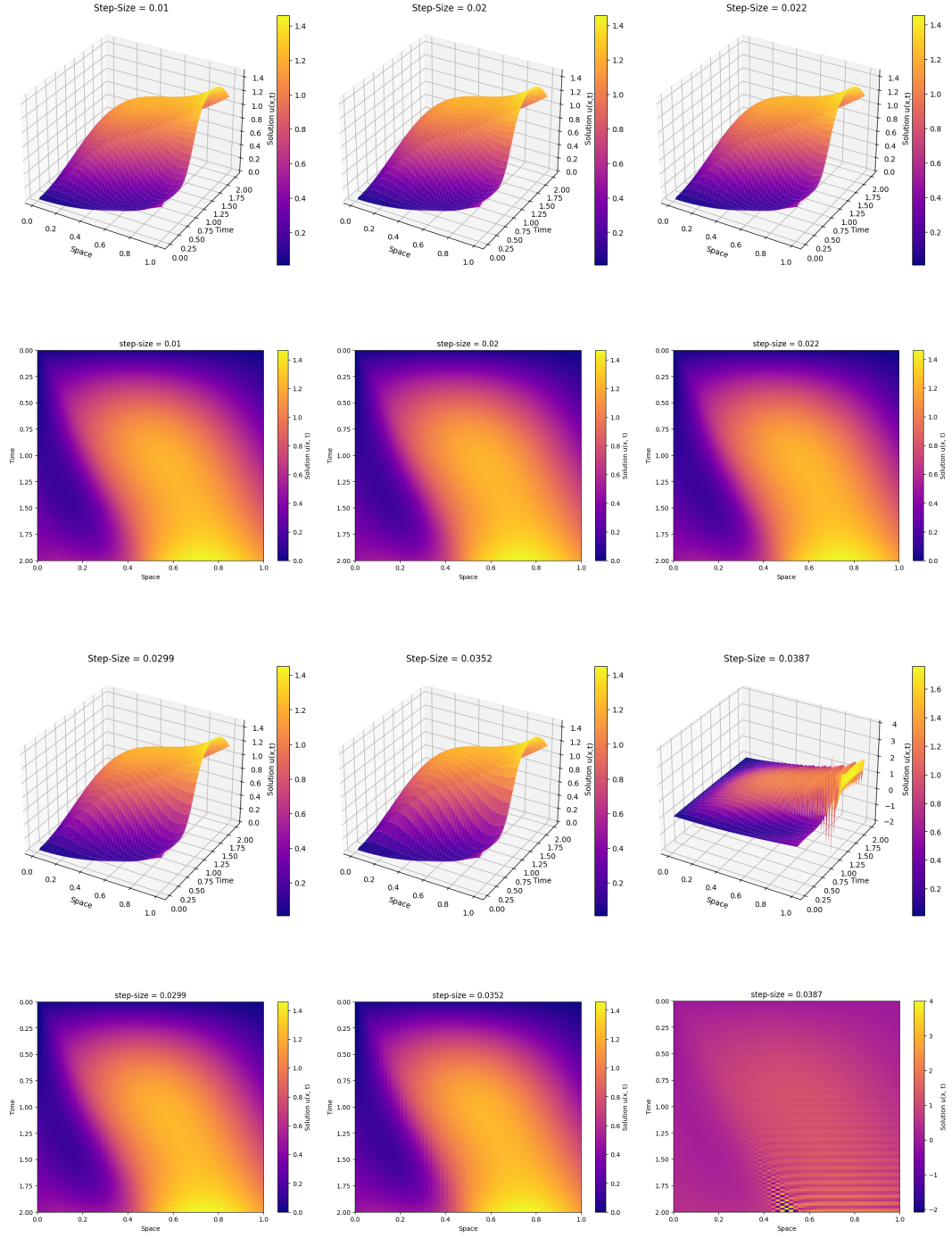


Figure 7.3: Comparison of numerical solutions for $m = 7, \phi_7(\Lambda_4), R_7(\Lambda_4) = 3.52$

7.1.3 Numerical Testing with Chebyshev Collocation Points

The data in Table 7.5 reveals that for the polynomial $\phi = \phi_7(\Lambda_3)$, there exists no scheme that ensures positivity. For all tested values of $N \in \{51, 56, 90, 100\}$, the corresponding entries are absent, indicating that no numerical scheme satisfies the required positivity conditions within the tested range of step sizes.

Moreover, the results in Table 7.8 show that for $h/\Delta x = 0.001724$ and 0.017238 positivity is preserved. The minimum value remains non-negative and the infinity norm is well-controlled below 1, indicating stable numerical behavior.

At $h/\Delta x = 0.036217$, positivity is lost as indicated by $\min(u) = -2.41 \times 10^{-1}$, although the solution remains numerically bounded with $\|u\|_\infty \approx 0.836$.

At $h/\Delta x = 0.036372$, positivity is violated and the solution exhibits catastrophic instability, with $\min(u)$ and $\|u\|_\infty$ both reaching magnitudes on the order of 10^{44} .

These results highlight the necessity of maintaining $h/\Delta x \leq R_{m,p}$ for positivity and for ensuring the stability and the reliability of the numerical scheme.

N	F	$h/\Delta x$	$\ u\ _\infty$	$\sigma(u)$	$\min(u)$
$(m = 7) \quad \phi = \phi_7(\Lambda_3)$					
51			—		
56			—		
90			—		
100			—		
$(m = 5) \quad \phi = \phi_5(\Lambda_4)$					
51	5100	3.89	1.791×10^{48}	3022	-1.791×10^{48}
56	5600	3.52	8.706×10^{40}	3388	-3.377×10^{40}
90	9000	2.20	2.727×10^0	1	-0.0728
100	10000	2.00	1.466×10^0	0	0.000
$(m = 7) \quad \phi = \phi_7(\Lambda_4)$					
51	5100	3.89	1.196×10^1	125	-9.664
56	5600	3.52	1.458×10^0	0	0.000
90	9000	2.20	1.462×10^0	0	0.000
100	10000	2.00	1.466×10^0	0	0.000

Table 7.5: Numerical results for different m values, $\Phi_m(\Lambda_p)$ with p Chebyshev collocation points

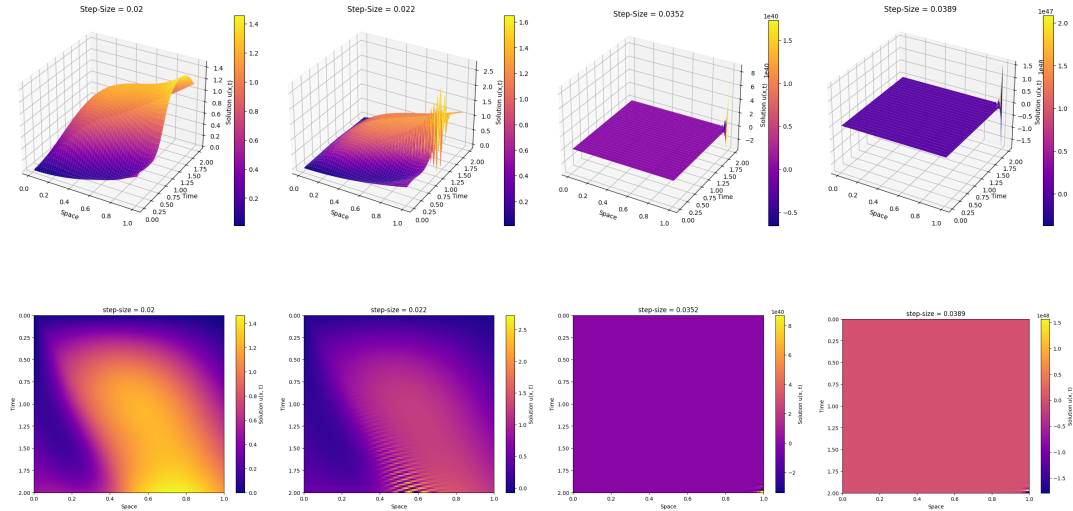


Figure 7.4: Numerical solutions for with 4 Chebyshev's collocation points for $m = 5, \phi_5(\Lambda_4)$ and $R_5(\Lambda_4) = 2$

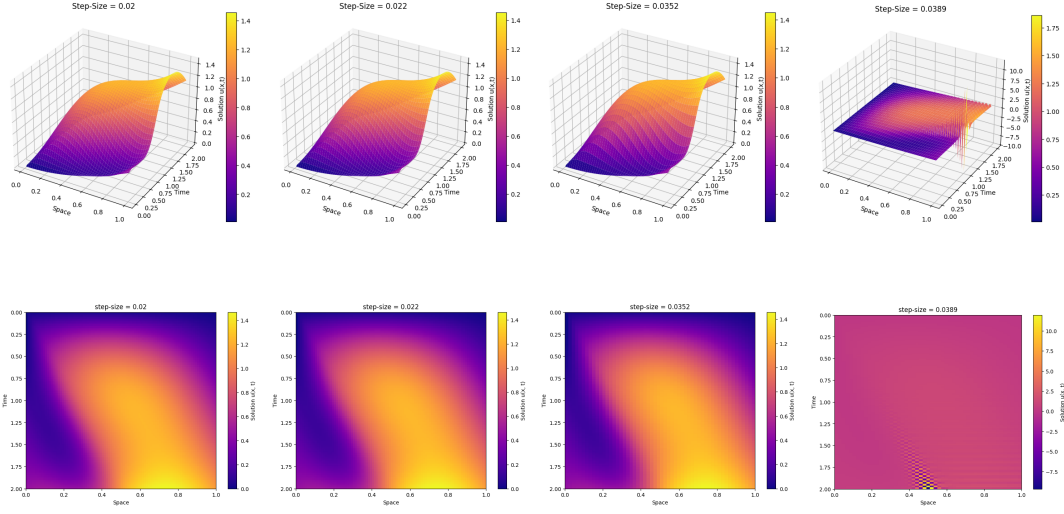


Figure 7.5: Numerical solutions for with 4 Chebyshev's collocation points for $m = 7$, $\phi_7(\Lambda_4)$ and $R_7(\Lambda_4) = 3.52$

7.2 Solar Thermal Storage Model

The dynamics of solar thermal storage systems can be modeled effectively using the one-dimensional heat equation with an external forcing term representing thermal input. Specifically, the governing equation is given by

$$\frac{\partial u}{\partial t} = k \frac{\partial^2 u}{\partial x^2} + 5e^{-10(x-0.5)^2} (\sin(2\pi t) + 1), \quad 0 < x < 1, \quad t > 0,$$

with initial and boundary conditions

$$u(x, 0) = \max(0, \sin(\pi x)), \quad u(0, t) = 0, \quad u(1, t) = 0.$$

Here, the domain is discretized using a second-order finite difference scheme, resulting in a uniform spatial grid spacing $\Delta x = 1/(N_x + 1) \approx 0.019608$ with $N_x = 50$ interior points. The discrete Laplacian matrix A associated with this discretization has constant diagonal elements $a_{ii} = -2/\Delta x^2$, yielding a maximum absolute diagonal elements of $\max |a_{ii}| = 5202$. Our tests were performed using the exponential integrator method with Legendre collocation points with $m = 7$ and $p = 4$.

For positivity preservation the time integration step size must satisfy the theoretical condition

$$h \leq \frac{R_{m,p}}{\max_{i=1,2,\dots,n} |a_{ii}|} = \frac{3.518}{5202} \approx 0.00067623,$$

where $R_{m,p} = 3.518$ is the method parameter. This condition ensures the positivity-preserving property of the numerical scheme for linear and inhomogeneous systems.

We examine the numerical solution behavior for three carefully chosen step sizes, $h = 0.000338$, which is half the theoretical threshold, $h = 0.000676$, exactly equal to the threshold, and $h = 0.000710$, slightly exceeding it. Table 7.6 summarizes the numerical outcomes for these choices. Step sizes of $h = 0.000338$ and $h = 0.000676$ clearly maintain non-negativity, confirming positivity and stability. However, a marginal violation at $h = 0.000710$ results in negative values and instability, underscoring the sensitivity of the method to slight deviations above the theoretical bound.

Step size h	Δx	$h/\Delta x$	$\min(u)$	$\ u\ _\infty$
0.000338	0.019608	0.017245	0.000000	0.837064
0.000676	0.019608	0.034490	0.000000	0.836420
0.000710	0.019608	0.036215	-1.021562	1.523811

Table 7.6: Positivity behavior for different step sizes.

Visualizations including a 3D surface plot and a heatmap (Figure 7.6) for the critical step size $h = 0.000676$ illustrate the evolution and preservation of positivity in the solution. These figures demonstrate the scheme's effectiveness and robustness when operating precisely at the theoretical boundary.

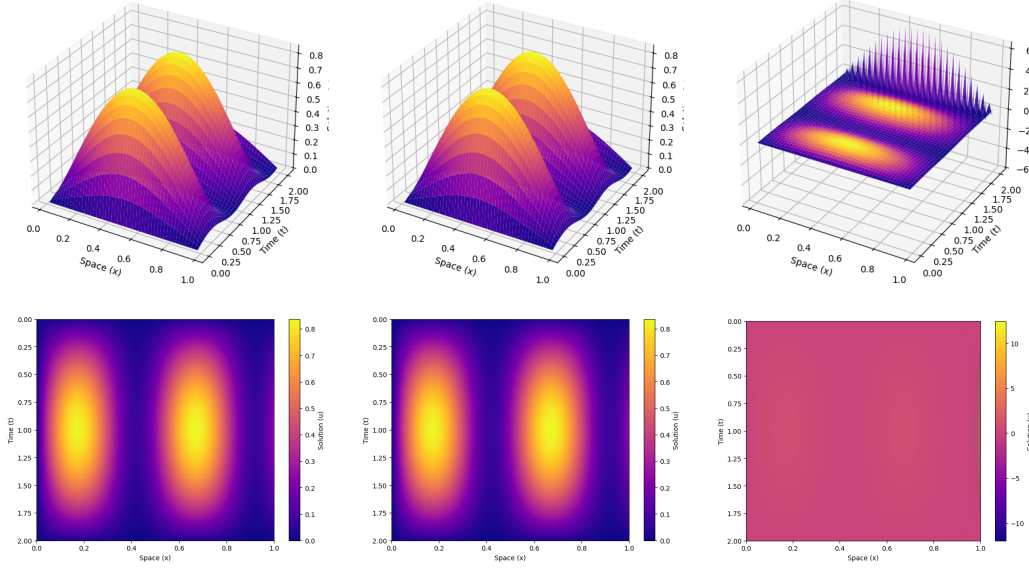


Figure 7.6: Solar Thermal Storage Model temperature distributions with $R_{m,p} = 3.518$ and $\Delta x = 0.019608$. The top row shows 3D surface plots, and the bottom row shows corresponding heatmaps for varying mesh sizes, (left) $h = 0.0000338$, (middle) $h = 0.000676$, and (right) $h = 0.00071$.

7.2.1 Positivity and Stability Examination

We analyze the numerical behavior of a positivity-preserving scheme applied to the one-dimensional heat equation with Gaussian forcing. The spatial domain $[0, 1]$ was discretized into $N_x = 50$ interior points, giving a uniform spacing $\Delta x = 1/(N_x + 1) \approx 0.019608$. The discrete Laplacian matrix A resulting from the finite-difference

discretization has diagonal elements $a_{ii} = -2/\Delta x^2$, hence $\max |a_{ii}| = 5202$. The theoretical positivity-preserving time-step restriction is given by

$$h \leq \frac{R_{m,p}}{\max |a_{ii}|} = \frac{3.518}{5202} \approx 0.00067623.$$

To examine the sensitivity of the numerical scheme to this condition, we performed simulations using three step sizes $h = 0.000338$, $h = 0.000676$, and a slightly larger step size $h = 0.000710$.

The results, summarized in Table 7.7, demonstrate clear differences in numerical behavior. The numerical solutions at step sizes $h = 0.000338$ and $h = 0.000676$ remain stable and physically realistic, with final maximum temperatures of approximately 0.251225 and 0.251771, respectively, and minimal values remaining positive. In contrast, the slightly increased step size $h = 0.000710$ resulted in severe instability, with a final maximum temperature of 975.233637 and a pronounced negative minimum temperature of -974.730523 , indicating a breakdown in positivity and stability.

h	$h/\Delta x$	Final Max Temp	Final Avg Temp	Final Min Temp
0.000338	0.017247	0.251225	0.158189	0.014351
0.000676	0.034494	0.251771	0.158533	0.014382
0.000710	0.036219	975.233637	0.158398	-974.730523

Table 7.7: Numerical results for different time-step sizes at final time, $\Delta x = 0.019608$, Max Temp Location=0.490196.

Plots corresponding to the stable cases ($h = 0.000338$ and $h = 0.000676$) show well-behaved solution profiles, whereas the unstable scenario ($h = 0.000710$) exhibits extreme oscillations, reinforcing the sensitivity of the scheme to the derived theoretical constraint. These visual observations complement and confirm the numerical data

presented in Table 7.6.

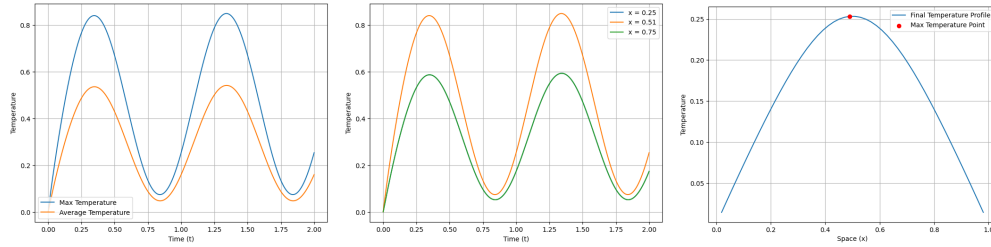


Figure 7.7: Temperature evolution and final distribution for $h_1 = 0.000034$. From left to right, (a) Maximum and average temperature over time; (b) Temperature at selected spatial points over time; (c) Final temperature distribution with the maximum temperature point marked.

Step Size $h_2 = 0.00033850$

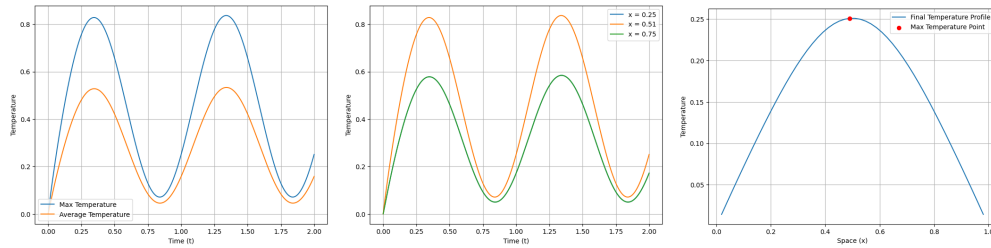


Figure 7.8: Temperature evolution and final distribution for $h_2 = 0.00033850$. From left to right, (a) Maximum and average temperature over time; (b) Temperature at selected spatial points over time; (c) Final temperature distribution with the maximum temperature point indicated.

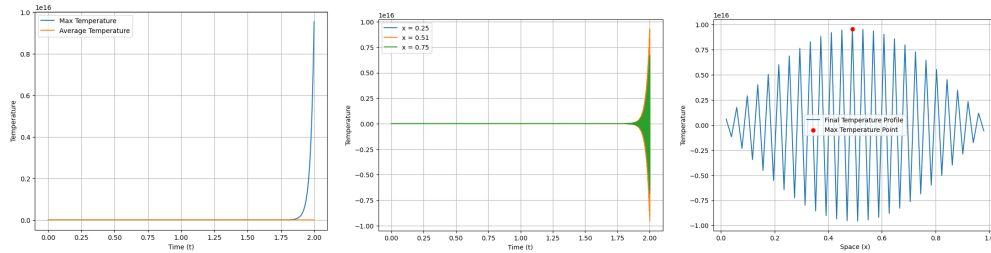


Figure 7.9: Temperature evolution and final distribution for $h_3 = 0.00071118$. From left to right, (a) Maximum and average temperature over time showing instability; (b) Temperature at selected spatial points over time with extreme oscillations; (c) Final temperature distribution showing divergence.

7.3 Transient Heat Conduction with Internal Heat Generation

We consider the one-dimensional transient heat conduction model with internal heat generation represented by a quadratic source

$$\frac{\partial u}{\partial t} = k \frac{\partial^2 u}{\partial x^2} + e^{-t} x^2 (L - x)^2, \quad 0 < x < 1, \quad t > 0,$$

subject to the initial and boundary conditions

$$u(x, 0) = 0, \quad u(0, t) = 0, \quad u(L, t) = 0.$$

This scenario models transient heating in a medium where the heat source peaks at the center and exponentially decays over time. The symmetric spatial profile ensures energy enters uniformly from the interior while dissipating at the boundaries.

We discretize the spatial domain using a second-order central difference scheme, yielding

$$\Delta x = \frac{1}{N_x + 1} \approx 0.019608, \quad N_x = 50.$$

The maximum absolute diagonal of the discrete Laplacian matrix is

$$\rho = \max |a_{ii}| = \frac{2}{\Delta x^2} \approx 5202.$$

According to the positivity-preserving theory, the time step h must satisfy

$$h \leq \frac{R_{m,p}}{\rho} = \frac{3.518}{5202} \approx 0.00067623.$$

To test this condition, we analyze the scheme's performance for

$$h = 0.000338 \text{ (half threshold),}$$

$$h = 0.000676 \text{ (exact threshold),}$$

$$h = 0.000710 \text{ (above threshold).}$$

The results are summarized in Table 7.8. For $h = 0.000338$ and $h = 0.000676$, the solution retains its positivity, thereby validating our theoretical predictions. However, at $h = 0.000710$, the minimum value becomes negative and the maximum norm increases sharply, indicating loss of stability and violation of positivity.

Step Size	Space Size (Δx)	Step/Space	$\min(u)$	$ u _\infty$
0.000338	0.019608	0.017263	0.000000e+00	4.432070e-03
0.000676	0.019608	0.034494	0.000000e+00	4.440618e-03
0.000710	0.019608	0.036219	-5.301407e-02	5.301407e-02

Table 7.8: Step-size versus space-size comparison with positivity indicators

Figures 7.10 and 7.11 illustrate these behaviors. For $h \leq 0.000676$, both the surface and heatmap visualizations remain smooth and strictly non-negative. In contrast, for $h = 0.000710$, the solution exhibits oscillations and a sharp breakdown in physical behavior. This highlights the necessity of step size control to preserve qualitative features in diffusion problems with time-varying sources.

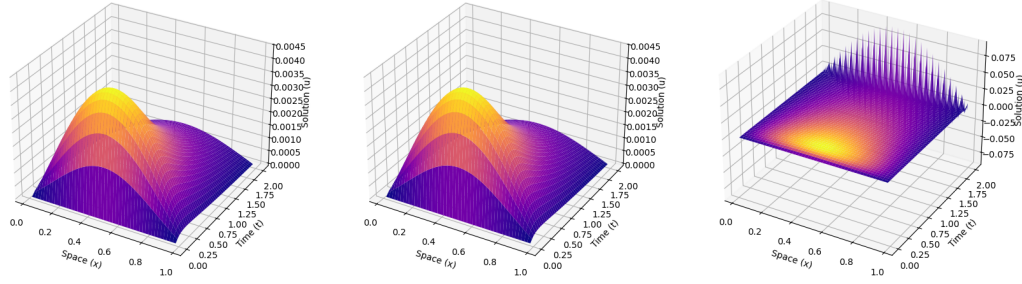


Figure 7.10: 3D surface plots of solution for $h = 0.000338$ (left), $h = 0.000676$ (middle), and $h = 0.000710$ (right)

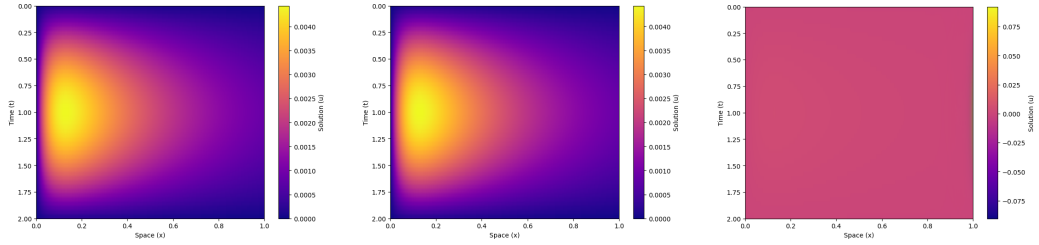


Figure 7.11: Heatmaps of temperature distribution for $h = 0.000338$ (left), $h = 0.000676$ (middle), and $h = 0.000710$ (right)

These results highlight the critical role of adhering to the theoretical time step constraint for preserving positivity and stability. The heatmap analysis in (7.11) specifically emphasizes that exceeding the threshold time step leads to numerical instability, even in scenarios where the forcing term and initial conditions support positivity under appropriate conditions.

7.4 Conclusion and Future Work

This thesis establishes a comprehensive framework for designing high-order exponential integrator schemes that preserve essential structural characteristics of the original system. The focus has been on deriving optimal positivity-preserving high-order exponential integrators for non-homogeneous linear problems using a generalized notion of optimal threshold factor. Applications to partial differential equations were examined in detail.

A central contribution of this work is the development of a new class of discrete orthogonal polynomials that shed light into the optimal threshold factor of any sequence of positive real numbers. These polynomials generalize classical families such as Poisson–Charlier, Meixner, and Krawtchouk, and their zeros provide critical spectral information necessary for bounding and computing optimal threshold factors. A computationally efficient algorithm based on Christoffel transformations is introduced, with complexity depending only on the polynomial order. This enabled practical computation of optimal threshold factors even for large numbers of stages.

The effectiveness of the proposed methods has been demonstrated through numerical experiments applied to representative partial differential equations. These experiments confirmed the accuracy, positivity preservation, and computational efficiency of the constructed schemes.

This work opens several directions for further investigation. The Christoffel transform-based algorithm developed in this thesis applies to general sequences and is not restricted to p -absolutely monotonic sequences; however, the associated theoretical anal-

ysis becomes significantly more intricate and will be the object of future investigation.

A natural extension of our framework involves replacing polynomial-based integrators with rational-function-based schemes. This generalization is expected to enhance both the flexibility and accuracy of the methods. Additionally, future research may focus on constructing optimal exponential integrators that preserve contractivity, which is especially relevant in modeling dissipative and energy-stable systems. Extending our work to exponential Runge-Kutta methods represents a highly ambitious undertaking.

Together, these directions highlight the potential for expanding the theory and application of structure-preserving exponential integrators in numerical analysis and scientific computing.

APPENDIX A

PROOFS

APPENDIX B

SUPPLEMENTARY MATERIAL

REFERENCES

- [1] L. Lóczi and D. Ketcheson, “Rational functions with maximal radius of absolute monotonicity,” *LMS Journal of Computation and Mathematics*, vol. 17, no. 1, pp. 159–205, 2014.
- [2] W. Wu, N. Liu, C. Huang, P. Zhang, and M. Liu, “A positivity-preserving lagrangian discontinuous galerkin scheme with exact riemann solver for gas-water compressible flows,” *International Journal for Numerical Methods in Fluids*, 2023.
- [3] H. Ranocha, “Shallow water equations: split-form, entropy stable, well-balanced, and positivity preserving numerical methods,” *GEM-International Journal on Geomathematics*, vol. 8, no. 1, pp. 85–133, 2017.
- [4] B. Ren, Z. Gao, Y. Gu, S. Xie, and X. Zhang, “A positivity-preserving and well-balanced high order compact finite difference scheme for shallow water equations,” *Communications in Computational Physics*, vol. 35, no. 2, pp. 524–552, 2024.
- [5] M. Z. Jacobson, A.-K. von Krauland, K. Song, and A. N. Krull, “Impacts of green hydrogen for steel, ammonia, and long-distance transport on the cost of meeting electricity, heat, cold, and hydrogen demand in 145 countries running on 100% wind-water-solar,” *Smart Energy*, vol. 11, p. 100106, 2023.

- [6] J. Akpan and O. Olanrewaju, “Sustainable energy development: History and recent advances,” *Energies*, vol. 16, no. 20, p. 7049, 2023.
- [7] R. J. Spiteri and S. J. Ruuth, “A new class of optimal high-order strong-stability-preserving time discretization methods,” *SIAM Journal on Numerical Analysis*, vol. 40, no. 2, pp. 469–491, 2002.
- [8] C. Jiang, J. Cui, X. Qian, and S. Song, “High-order linearly implicit structure-preserving exponential integrators for the nonlinear schrödinger equation,” *Journal of Scientific Computing*, vol. 90, no. 1, p. 66, 2022.
- [9] A. Ostermann, M. Thalhammer, and W. Wright, “A class of explicit exponential general linear methods,” *BIT Numerical Mathematics*, vol. 46, pp. 409–431, 2006.
- [10] S. J. Ruuth and R. J. Spiteri, “High-order strong-stability-preserving runge–kutta methods with downwind-biased spatial discretizations,” *SIAM Journal on Numerical Analysis*, vol. 42, no. 3, pp. 974–996, 2004.
- [11] W. E. Schiesser, *The numerical method of lines: integration of partial differential equations*. Elsevier, 2012.
- [12] M. Hochbruck and A. Ostermann, “Exponential integrators,” *Acta Numerica*, vol. 19, pp. 209–286, 2010.
- [13] P. Brenner, M. Crouzeix, and V. Thomée, “Single step methods for inhomogeneous linear differential equations in banach space,” *RAIRO. Analyse numérique*, vol. 16, no. 1, pp. 5–26, 1982.

- [14] C. Bolley and M. Crouzeix, “Conservation de la positivité lors de la discrétisation des problèmes d’évolution paraboliques,” *RAIRO Analyse Numérique*, vol. 12, no. 3, pp. 237–245, 1978.
- [15] R. S. Varga, “Nonnegatively posed problems and completely monotonic functions,” *Linear Algebra Appl*, vol. 1, no. 3, pp. 329–347, 1968.
- [16] S. Gottlieb, C.-W. Shu, and E. Tadmor, “Strong stability preserving high-order time discretization methods,” *SIAM Review*, vol. 43, pp. 89–112, 2001.
- [17] I. Higueras, “On strong stability preserving time discretization methods,” *Journal of Scientific Computing*, vol. 21, no. 2, pp. 193–223, 2004.
- [18] L. Isherwood, Z. J. Grant, and S. Gottlieb, “Strong stability preserving integrating factor runge-kutta methods,” *SIAM Journal on Numerical Analysis*, vol. 56, no. 6, pp. 3276–3307, 2018.
- [19] D. I. Ketcheson, “Computation of optimal monotonicity preserving general linear methods,” *Mathematics of Computation*, vol. 78, no. 267, pp. 1497–1513, 2009.
- [20] H. Zhang, J. Yan, X. Qian, and S. Song, “Numerical analysis and applications of explicit high order maximum principle preserving integrating factor runge-kutta schemes for allen-cahn equation,” *Applied Numerical Mathematics*, vol. 161, pp. 372–390, 2021.
- [21] E. Hairer and C. Lubich, “Large-stepsize integrators for charged particles in a strong magnetic field,” in *AIP Conference Proceedings*, vol. 2849, no. 1. AIP Publishing, 2023.

- [22] D. Cohen and E. Hairer, “Linear energy-preserving integrators for poisson systems,” *BIT Numerical Mathematics*, vol. 51, no. 1, pp. 91–101, 2011.
- [23] D. I. Ketcheson, C. B. Macdonald, and S. Gottlieb, “Optimal implicit strong stability preserving runge-kutta methods,” *Applied Numerical Mathematics*, vol. 59, no. 2, pp. 373–392, 2009.
- [24] N. Bosch, P. Hennig, and F. Tronarp, “Probabilistic exponential integrators,” *arXiv preprint arXiv:2305.14978*, 2023.
- [25] J. Li and X. Jin, “Structure-preserving exponential wave integrator methods and the long-time convergence analysis for the klein-gordon-dirac equation with the small coupling constant,” *Numerical Methods for Partial Differential Equations*, vol. 39, no. 4, pp. 3375–3416, 2023.
- [26] Q. Zhang and Y. Chen, “Fast sampling of diffusion models with exponential integrator,” *arXiv preprint arXiv:2204.13902*, 2022.
- [27] N. Bosch, P. Hennig, and F. Tronarp, “Probabilistic exponential integrators,” *Advances in Neural Information Processing Systems*, vol. 36, pp. 40 450–40 467, 2023.
- [28] F.-X. Briol, C. J. Oates, M. Girolami, M. A. Osborne, and D. Sejdinovic, “Probabilistic integration,” *Statistical Science*, vol. 34, no. 1, pp. 1–22, 2019.
- [29] N. Krämer, N. Bosch, J. Schmidt, and P. Hennig, “Probabilistic ode solutions in millions of dimensions,” in *International Conference on Machine Learning*. PMLR, 2022, pp. 11 634–11 649.

- [30] I. Higueras, “Representations of runge–kutta methods and strong stability preserving methods,” *SIAM Journal on Numerical Analysis*, vol. 43, no. 3, pp. 924–948, 2005.
- [31] S. Ruuth, “Global optimization of explicit strong-stability-preserving runge-kutta methods,” *Mathematics of Computation*, vol. 75, no. 253, pp. 183–207, 2006.
- [32] S. N. Bernstein, “Sur les fonctions absolument monotones,” *Acta Mathematica*, vol. 52, pp. 1–66, 1928.
- [33] J. F. B. M. Kraaijevanger, “Absolute monotonicity of polynomials occurring in the numerical solution of initial value problems,” *Numerische Mathematik*, vol. 48, no. 3, pp. 303–322, 1986.
- [34] —, “Contractivity of runge-kutta methods,” *BIT Numerical Mathematics*, vol. 31, no. 3, pp. 482–528, 1991.
- [35] A. Gerisch and R. Weiner, “The positivity of low-order explicit runge-kutta schemes applied in splitting methods,” *Computers & Mathematics with Applications*, vol. 45, no. 1-3, pp. 53–67, 2003.
- [36] R. Ait-Haddou, “Computation of optimal linear strong stability preserving methods via adaptive spectral transformations of poisson–charlier measures,” *Journal of Scientific Computing*, vol. 88, p. 66, 2021.
- [37] S. Karlin and G. Szegő, “On certain determinants whose elements are orthogonal polynomials,” *Journal d’Analyse Mathématique*, vol. 8, no. 1, pp. 1–157, 1960.

- [38] L. Ramshaw, “Blossoms are polar forms,” *Computer Aided Geometric Design*, vol. 6, no. 4, pp. 323–358, 1989.
- [39] D. Gallant, “An implementation of christoffel’s theorem in the theory of orthogonal polynomials,” *Mathematics of Computation*, vol. 25, pp. 111–113, 1971.
- [40] J. Hersch, “Contribution à la méthode des équations aux différences,” *Zeitschrift für angewandte Mathematik und Physik (ZAMP)*, vol. 9, pp. 129–180, 1958.
- [41] S. M. Cox and P. C. Matthews, “Exponential time differencing for stiff systems,” *Journal of Computational Physics*, vol. 176, no. 2, pp. 430–455, 2002.
- [42] N. J. Higham, “Functions of matrices: theory and computation,” 2008.
- [43] R. Ait-Haddou and M.-L. Mazure, “The fundamental blossoming inequality in chebyshev spaces—i: Applications to schur functions,” *Foundations of Computational Mathematics*, vol. 18, pp. 135–158, 2018.
- [44] R. Ait-Haddou, W. Herzog, and T. Nomura, “Complex bézier curves and the geometry of polygons,” *Computer Aided Geometric Design*, vol. 27, no. 7, pp. 525–537, 2010.
- [45] I. Area, D. Dimitrov, E. Godoy, and V. Paschoa, “Zeros of classical orthogonal polynomials of a discrete variable,” *Mathematics of Computation*, vol. 82, no. 282, pp. 1069–1095, 2013.

- [46] D. V. Widder, “The inversion of the laplace integral and the related moment problem,” *Transactions of the American Mathematical Society*, vol. 36, no. 1, pp. 107–200, 1934.
- [47] T.-J. Stieltjes, “Recherches sur les fractions continues,” in *Annales de la Faculté des sciences de Toulouse: Mathématiques*, vol. 8, no. 4, 1894, pp. J1–J122.
- [48] J. Farkas, “Theorie der einfachen ungleichungen.” *Journal für die reine und angewandte Mathematik (Crelles Journal)*, vol. 1902, no. 124, pp. 1–27, 1902.
- [49] L. Pochhammer, “Ueber hypergeometrische functionen nter ordnung.” *Journal für die reine und angewandte Mathematik (Crelles Journal)*, vol. 1870, no. 71, pp. 316–352, 1870.
- [50] A. F. Nikiforov, V. B. Uvarov, S. K. Suslov, A. F. Nikiforov, V. B. Uvarov, and S. K. Suslov, *Classical orthogonal polynomials of a discrete variable*. Springer, 1991.
- [51] R. S. Costas-Santos and J. Sánchez-Lara, “Orthogonality of q-polynomials for non-standard parameters,” *Journal of Approximation Theory*, vol. 163, no. 9, pp. 1246–1268, 2011.
- [52] D. Dominici, S. J. Johnston, and K. Jordaan, “Real zeros of ${}_2F_1$ hypergeometric polynomials,” *Journal of Computational and Applied Mathematics*, vol. 247, pp. 152–161, 2013.
- [53] W. Mitkowski, “Dynamical properties of metzler systems,” *Bulletin of the Polish Academy of Sciences: Technical Sciences*, vol. 56, no. 4, 2008.

- [54] Z. Sun, *Switched linear systems: control and design*. Springer Science & Business Media, 2006.
- [55] A. Bátkai, M. K. Fijavz, and A. Rhandi, “Positive operator semigroups: From finite to infinite dimensions, volume 257 of,” *Operator Theory: Advances and Applications*.
- [56] R. S. Varga, “Iterative analysis,” *New Jersey*, vol. 322, p. 24, 1962.

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