VILNIUS UNIVERSITY

FACULTY OF MATHEMATICS AND INFORMATICS

MASTERS IN MATHEMATICS

Master thesis

M-matrices, Chebyshev polynomials and applications for finite difference schemes

”M-matricos, Čebyševo polinomai ir taikymas baigtinių skirtumų schemoms”

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Vilnius
2025

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Acknowledgements

I am deeply grateful to my supervisor Dr. Artūras Stikonas, for his invaluable guidance, patience, and unwavering support throughout the course of this research. His expertise, insightful advice, and constructive feedback significantly shaped both the theoretical foundation and practical development of this work. I truly appreciate the time and effort he devoted to reviewing my progress, offering encouragement during challenging moments, and fostering an environment of academic curiosity and rigor that made this journey both rewarding and intellectually enriching.

I would also like to thank my friends and fellow students for their constant encouragement, stimulating discussions, and camaraderie that made the academic journey more enjoyable and less stressful. Their presence provided both motivation and meaningful support along the way.

Finally, I am profoundly thankful to my family for their unconditional love, endless patience, and unwavering belief in me. Their emotional support and encouragement have been the foundation that sustained me through every stage of this journey.

Santrauka

Šiame tyrime sukuriamas pagrindas, kuris sujungia M-matricų teoriją ir Čebyšovo daugianarius siekiant pagerinti baigtinių skirtumų metodų stabilumą ir tikslumą. Naudojame pagrindines M-matricų savybes – invertuojamumą, neigiamus ne įstrižainės elementus ir įstrižaininį dominavimą – kad užtikrintume stabilią diskretizaciją, kuri patikimai konverguoja. Čebyšovo daugianariai padeda pagerinti spektrinius aproksimavimus, sumažinti osciliacijas ir paspartinti sprendiklius. Šis derinys sprendžia stabilumo problemas esant staigiems gradientams ar blogai sąlygotiems sistemoms. Analizė ir eksperimentai rodo, kad metodas suteikia geresnes paklaidų ribas, mažesnį jautrumą tinklo pasirinkimui ir didesnį efektyvumą. Bandymai su ribinėmis sritimis ir aukštesnių dimensijų PDE patvirtina šio pagrindo praktinę vertę patikimam sudėtingų reiškinių modeliavimui, parodant, kaip matricų algebros ir daugianarių metodų sintezė pagerina skaitinius metodus.
keywords: M-matricos, Čebyšovo daugianariai, Eliptinės lygtys, Kronekerio sandauga, Puasono lygtis

Abstract

This study develops a framework that combines M-matrix theory and Chebyshev polynomials to improve the stability and accuracy of finite difference methods. We use key M-matrix traits invertibility, non-positive off-diagonals, and diagonal dominance to ensure stable discretizations that converge reliably. Chebyshev polynomials help improve spectral approximations, reduce oscillations, and speed up solvers. This combined approach tackles stability issues in problems with steep gradients or ill-conditioned systems. Analysis and experiments show it delivers better error bounds, less sensitivity to grid choice, and higher efficiency. Tests on boundary layers and high-dimensional PDEs confirm the framework's practical value for robustly simulating complex phenomena, demonstrating how merging matrix algebra and polynomial techniques advances numerical methods.

keywords: M-matrices, Chebyshev polynomials, Elliptic Equations, Kronecker Product, Poisson Equation

Chapter 1

Introduction

Matrix theory and numerical approximation techniques are foundational to solving large-scale systems arising in scientific computing, particularly for partial differential equations (PDEs). Among these, M-matrices a class of matrices with non-positive off-diagonal entries and positive principal minors play a pivotal role due to their unique spectral properties and guarantees of stability in iterative methods. Simultaneously, Chebyshev polynomials offer a powerful tool for accelerating iterative solvers, leveraging their minimax properties to optimize convergence rates. This thesis bridges these two domains, developing novel theoretical connections and computational frameworks that exploit M-matrix structures through Chebyshev polynomial-based algorithms.

The interplay between M-matrices and Chebyshev polynomials remains underexplored despite their complementary strengths: M-matrices ensure solvability and monotonicity in discretized PDE systems, while Chebyshev polynomials provide near-optimal approximation for eigenvalue-based iterations. We address this gap by characterizing the spectral radius of M-matrix splittings to establish convergence criteria, and designing Chebyshev-accelerated solvers that outperform classical methods in both speed and robustness. Our approach rigorously combines matrix analysis (e.g, Perron-Frobenius theory) with polynomial approximation techniques, yielding algorithms with provable efficiency gains for sparse linear systems.

Relevance and Motivation: Solving large systems of linear equations efficiently is crucial in computational science and engineering, especially when simulating complex physical phenomena like heat transfer, fluid flow, or structural mechanics using finite difference methods. These simulations often generate large, sparse linear systems derived from discretizing Partial Differential Equations (PDEs), particularly elliptic PDEs which model steady-state or equilibrium behaviors. Solving these systems can be computationally very expensive, demanding significant time and resources. Developing faster, more robust iterative solvers and preconditioners is therefore a critical ongoing challenge to enable larger, more complex, and more accurate simulations.

Research Problems and Objectives: While M-matrices frequently arise naturally in these finite difference discretizations (especially for elliptic PDEs) and possess beneficial inherent properties, and while Chebyshev polynomials are renowned for their ability to accelerate iterative methods based on spectral bounds, the deep theoretical connections and optimal synergy between these two concepts specifically within this context are not always fully exploited or clearly articulated. The core problems this thesis addresses are: How can the specific spectral properties of M-matrices be leveraged most effectively? How can Chebyshev polynomials, uniquely defined for matrices with known eigenvalue bounds, be optimally constructed and applied to M-matrices? How does this combination translate concretely into improved numerical methods for practical finite difference schemes? The primary objectives are: To rigorously explore the theoretical links between M-matrix properties and the design/behavior of Chebyshev polynomials for iterative methods. To develop and analyze efficient iterative solvers and preconditioners based on this M-matrix/Chebyshev combination. To demonstrate how these methods significantly accelerate convergence and reduce computational cost for elliptic PDEs solved via finite differences. To provide practical insights into enhancing the stability and efficiency of these critical computations.

Brief Description of Methodology: This research employed a blend of theoretical analysis and numerical experimentation. Key M-matrix properties (like inverse positivity and eigenvalue location) were reviewed and utilized to establish reliable spectral bounds. The theory behind Chebyshev polynomials of matrices was investigated, focusing on their construction, uniqueness, and optimal minimization properties given known eigenvalue intervals typical of M-matrices. Based on this foundation, novel iterative schemes and preconditioning strategies were designed specifically leveraging the synergy between M-matrix structure and Chebyshev approximation. The performance and convergence characteristics of these methods were then rigorously tested using benchmark elliptic PDE problems discretized with finite differences.

Summary of Key Results: This work has established a clear theoretical framework connecting the spectral properties of M-matrices with the construction and effectiveness of Chebyshev polynomials for iterative solvers. Efficient algorithms have been developed that combine these concepts, resulting in significantly accelerated convergence rates compared to standard methods. The resulting solvers and preconditioners have demonstrated a substantial reduction in computational cost (in terms of iteration count and time) for solving large sparse systems from finite difference discretizations of elliptic PDEs. Furthermore, the methods have shown improved stability characteristics in practical computations.Numerical methods for solving partial differential equations (PDEs) rely heavily on robust mathematical tools to balance accuracy, stability, and computational efficiency. Among these tools, and Chebyshev polynomials play pivotal roles in addressing challenges inherent to finite difference schemes. M-matrices a class of invertible matrices with non-positive off-diagonal entries and non-negative inverse are foundational in ensuring numerical stability, particularly for discretized elliptic PDEs, as their properties guarantee solutions remain physically meaningful and converge reliably. Complementing this, Chebyshev polynomials, renowned for their minimal oscillation and optimal approximation properties on interval boundaries, excel in mitigating errors like Runge's phenomenon and accelerating iterative solvers through spectral techniques. When integrated into finite difference frameworks, these polynomials enhance grid resolution near critical regions (boundary layers) and optimize preconditioners for large linear systems. Together, M-matrices and Chebyshev polynomials form a synergistic toolkit, enabling high-precision simulations in fields ranging from fluid dynamics to materials science. This interplay underscores their enduring relevance in modern computational science, where demands for scalable, stable, and efficient algorithms continue to grow alongside increasingly complex Multiphysics problems.

In Section 3, we discuss about mathematical background in which we study about basic of Matrices, M-matrices, Chebyshev polynomials and kronecker product. In Section 4, we discuss about discretization of elliptic equations using finite difference with nonlocal boundary conditions. In Section 5, we discuss about generalized finite difference solution for the 2D poisson equation, Inversion of Block tridiagonal matrices using chebyshev polynomials, inversion of block tridiagonal matrices using kronecker product and eigenvalue decomposition and applications of M-matrices. In Section 6, we discuss about conclusions and results.

Chapter 2

Literature Review

Reliable numerical methods for PDEs require balancing accuracy, stability, and speed. M-matrices (invertible matrices with non-positive off-diagonals and non-negative inverses) ensure stability for discretized elliptic PDEs, guaranteeing meaningful, convergent solutions. Chebyshev polynomials provide excellent approximation near boundaries and help avoid errors like the Runge phenomenon while accelerating solvers. While combining M-matrices and Chebyshev polynomials within finite difference methods has been explored, their full synergy and benefits are not fully developed. This research builds on existing work by rigorously linking M-matrix spectral properties to optimal Chebyshev polynomials for faster solvers, aiming to significantly boost convergence and efficiency for large sparse PDE systems.

Numerous studies have addressed the numerical treatment of elliptic partial differential equations (PDEs) and their boundary conditions. Forsythe-Wasow[11] employed the finite element method (FEM) to solve boundary value problems with diverse boundary conditions, demonstrating that discretization reduces such problems to linear algebraic systems. Similarly, Larson and Bengzon [23] developed finite element approaches for 2D PDEs, emphasizing variational formulations and piecewise linear approximations. Karakashian and Pascal [20] advanced this field by introducing residual-based error estimators for discontinuous Galerkin methods applied to elliptic problems with mixed Dirichlet-Neumann boundary conditions, ensuring adaptive refinement achieved target error bounds. Mitchell [29] contributed parametrized 2D elliptic test problems to benchmark adaptive grid refinement algorithms, incorporating singularities and other computational challenges. Hayek and Ackerer [16] validated numerical methods through synthetic cases, such as central inclusion problems, successfully reconstructing interface geometries. In the context of nonlocal boundary conditions (NBCs), Saharian et al. [37] analyzed vacuum expectation values for scalar fields under NBCs on geometric configurations like parallel plates. D'Elia and Yu [8] and Scott and Du [39] independently proposed techniques to convert local boundary conditions into nonlocal volume constraints for Poisson and peridynamic models, leveraging local solutions to approximate nonlocal data. Zorumski et al. [48] formulated NBCs for acoustic wave propagation in ducts, implementing constant matrix operators at computational boundaries. Nonlocal boundary conditions often involve integro-differential equations with position-dependent kernels, which vanish at boundaries to ensure consistency with classical local conditions in the vanishing horizon limit (Anonymous, n.d.). These methods face challenges in preserving structural matrix properties during discretization. For instance, Varga [44] established foundational M-matrix theory, highlighting its role in solving sparse linear systems iteratively. Grassi and Marino [14] extended M-theory matrix models to include non-perturbative corrections beyond the 't Hooft expansion. Chebyshev polynomials have been widely applied in numerical methods across various studies. Horner [18] utilized these polynomials to derive accurate numerical solutions for ordinary and partial differential equations, while also generalizing formulae for computing function and derivative values. Building on these foundations, Hu and Ji [15] later proposed an adaptive spatial partitioning method near asteroids using spherical coordinates, employing Chebyshev polynomial interpolation to model gravitational acceleration within subdivided regions. Subsequent work by Oboyi et al. [10] presented a modified rational interpolation approach for solving initial value problems, validating its efficacy through three numerical test cases. In more recent developments, Hubert and Singer [6] introduced a deterministic algorithm to reconstruct functions composed of linear combinations of up to *r* Chebyshev polynomials, requiring only *r* and a bounded number of function evaluations. The authors subsequently expanded this work (Hubert and Singer, 2021) by creating a sparse interpolation algorithm for similar Chebyshev-based function representations, further optimizing evaluation requirements. In studies of Chebyshev-based numerical methods, researchers highlighted distinct advantages and limitations. Lovetskiy et al. [25] implemented a spectral collocation method for solving two-point boundary value problems for second-order differential equations by representing solutions as expansions in Chebyshev polynomials. Similarly, Mead and Renaut [27] found that while the Chebyshev pseudospectral method provided spectral accuracy for integrating partial differential equations with spatial derivatives of order nn, it required time steps approximately proportional to $N-2$ where NN represented the number of spatial modes. Huang et al.[17] demonstrated computational efficiency improvements, showing that Chebyshev segmentation required fewer points than average segmentation to achieve equivalent accuracy, thereby reducing computational demands. Meanwhile, Zakharov and Zimin [47] noted that the Chebyshev iterative method was optimal in convergence rate for systems with self-adjoint and positive-definite matrices, though its applicability depended on prior knowledge of the matrix spectrum boundaries. Collectively, these studies underscored the trade-offs between accuracy, efficiency, and practical constraints in Chebyshev-based approaches.

Spectral analysis of discretized systems has also garnered attention. Lim et al. [24] surveyed spectral theories for nonnegative tensors, addressing eigenvalue problems and applications in Markov chains and quantum entanglement. Kwok et al.[22] demonstrated that gradient descent algorithms achieve linear convergence for matrices with spectral gaps, while Mazko [26] developed matrix-based methods for stability analysis in dynamic systems. Roach et al. [36] reviewed matrix techniques for molecular spectral data, emphasizing steady-state and dynamic measurements. In thermal and electromagnetic applications, Xu [46] conducted a comprehensive review of finite volume (FVM) and finite difference (FDM) methods for analyzing axial flux permanent magnet (AFPM) machines, detailing their advantages and limitations. Poljak et al. [33],[34] applied FDM and FEM to model magnetohydrodynamics (MHD) in fusion research and quantum nanostructures. Geiser (2009) introduced a second-order operator-splitting method for convection-reaction equations, combining analytical and numerical solutions for improved accuracy. Shi et al. [40]compared six discretization methods for electrolyte diffusion, evaluating their temporal and frequency-domain precision. Korman and Schmidt [21] simplified the Dirichlet problem by reducing the number of particles in the solution to three, streamlining computational efforts. Earlier foundational work by Varga [43] introduced matrix methods for parabolic partial differential equations (PPDEs), where acceleration parameters were rigorously estimated and solutions to elliptic difference equations were derived. Building on these frameworks, Assanova [1] proposed a novel approach to nonlocal problems involving integral conditions, addressing challenges in boundary value analysis. Similarly, Pereira and Rossi [31] investigated nonlocal problems within perforated domains, focusing on equations with non-singular kernels to generalize applicability across discontinuous media. Collectively, these studies advanced methodologies for solving differential equations, emphasizing efficiency and adaptability to complex geometries.

Despite these advances, gaps persist in analyzing how nonlocal boundary conditions affect M-matrix properties and spectral behavior. Earlier works, such as Taylor [42] and Bigatti and Susskind [5], explored matrix models in theoretical physics but did not address numerical PDE contexts. This review underscores the need for frameworks that preserve M-matrix structures under NBCs while enabling robust spectral analysis a gap addressed in the present work.

Chapter 3

Mathematical Background

This chapter introduces the foundational mathematical concepts necessary for analyzing M-matrices in the context of two-dimensional elliptic partial differential equations (PDEs) with nonlocal boundary conditions. We review elliptic PDEs, nonlocal boundary conditions, discretization methods, and the properties of M-matrices relevant to spectral and numerical analysis.

3.0.1 Matrices

This thesis begins by introducing the essential matrix theory concepts and results relevant to our analysis. Let $\mathbb{C}^+$ denote the set of complex numbers whose real parts are strictly positive, that is $\mathbb{C}^+ := \{z \in \mathbb{C} \mid \text{Re}(z) > 0$. A complex matrix of size $n \times m$ is denoted by **A** $= (a_{ij})$, where each entry $a_{ij} \in \mathbb{C}$. If all elements of **A** are real, then **A** $\in \mathbb{R}^{n\times m}$. Column vectors are written in the form **V** $= (v_1, \dots, v_n)^\top \in \mathbb{R}^{n\times 1} \equiv \mathbb{R}^n$.
An identity matrix is a square matrix where all diagonal elements are **1** and all off-diagonal elements are **0**. It is denoted by **I**. A zero matrix is a matrix in which all the elements are zero. It is denoted as **O**. Apart from the standard matrix multiplication **AB** $= \left(\sum_{j=1}^{m} a_{ij} b_{jl}\right) \in \mathbb{C}^{n\times k}$, where **A** $\in \mathbb{C}^{n\times m}$ and **B** $\in \mathbb{C}^{m\times k}$, the Kronecker product will also be utilized as a block matrix **A**$\otimes$**B** $= (a_{ij}B) \in \mathbb{C}^{n_1 n_2 \times m_1 m_2}$, where **A** $\in \mathbb{C}^{n_1\times m_1}$ and **B** $\in \mathbb{C}^{n_2\times m_2}$. A transformation that turns a matrix into a vector is called vectorization. The vectorization process for a matrix A is defined as: **V** $= (V_1, \dots, V_k)^\top = \text{vec}(\mathbf{A}) := (a_{11}, \dots, a_{n1}, a_{12}, \dots, a_{n2}, \dots, a_{1m}, \dots, a_{nm})^\top$, where $k = nm$. The set of all eigenvalues $\lambda_1, \dots, \lambda_n$ of a matrix **A** $\in \mathbb{C}^{n\times n}$ is known as the spectrum, denoted as $\sigma(\mathbf{A})$ The spectral radius of **A** is defined as $\rho(\mathbf{A}) := \max_{i=1,\dots,n} |\lambda_i|$. The norms used for vectors and matrices are as follows:

$$\|\mathbf{A}\|_2 := \left(\rho(AA^*)\right)^{1/2}, \quad \|\mathbf{A}\|_\infty := \max_{i=1,\dots,n} \sum_{j=1}^{m} |a_{ij}|,$$

$$\|\mathbf{V}\|_2 := \left(\sum_{i=1}^{n} |v_i|^2\right)^{1/2}, \quad \|\mathbf{V}\|_\infty := \max_{i=1,\dots,n} |v_i|,$$

A square matrix $\mathbf{A} \in \mathbb{C}^{n\times n}$ is said to be *irreducible* if there does not exist a permutation matrix **P** such that

$$\mathbf{PAP^{-1}} = \begin{pmatrix} \mathbf{A}_1 & \mathbf{A}_2 \\ \mathbf{0} & \mathbf{A}_3 \end{pmatrix},$$

where the square matrices $\mathbf{A_1}$ and $\mathbf{A_3}$ are non-trivial. A matrix $\mathbf{A} \in \mathbb{C}^{n\times n}$ is said to be *diagonally dominant* (also known as weak diagonal dominance) if:

$$|a_{ii}| \geq \sigma_i, \quad \sigma_i := \sum_{j\neq i} |a_{ij}|, \quad \forall i.$$

If the inequality is strict (i.e., $|a_{ii}| > \sigma_i$ for all i), the matrix is called strictly diagonally dominant. Additionally, if **A** is irreducible and there exists at least one index k for which $|a_{kk}| > \sigma_k$, then **A** is referred to as *irreducibly diagonally dominant*.

3.0.1.1 Theorem ([13])**.** *The set D contains all of the eigenvalues of* $\mathbf{A} \in \mathbb{C}^{n\times n}$*, which means that* $\sigma(\mathbf{A}) \subset D$*.*

Furthermore, the Gershgorin disks connected to $\mathbf{A}^\top$ also include the eigenvalues of A.

Nonnegative matrices. The Perron–Frobenius theorem in matrix theory states that a real square matrix with positive entries has a singular eigenvalue of highest magnitude and that eigenvalue is real. It was demonstrated by O. Perron [32] and G. Frobenius [12].

If $0 \leq \mathbf{A} \leq \mathbf{B}$, then $\rho(\mathbf{A}) \leq \rho(\mathbf{B})$ holds true. Furthermore, if $\mathbf{A} \neq \mathbf{B}$ and **B** is irreducible, then the inequality is strict. The spectral radius of **A** is less than the spectral radius of **B**.

3.0.1.2 Theorem ([45, Theorem 2.7],[2, Theorem 4.11],[3, Theorem 2.1.4])**.** *Let* $0 \leq \mathbf{A} \in \mathbb{R}^{n\times n}$ *be an* irreducible matrix*. Then the following properties hold:*

(i) The matrix **A** *possesses a positive real eigenvalue* $r_{\mathbf{A}}$ *that coincides with its spectral radius* $\rho(\mathbf{A})$*.*

(ii) A corresponding positive eigenvector $\mathbf{V} > 0$ *is linked to* $r_{\mathbf{A}}$*.*

(iii) The value of $r_{\mathbf{A}}$ *rises whenever any entry of* **A** *is increased.*

(iv) The simple eigenvalue of **A** *is* $r_{\mathbf{A}}$*.*

All other eigenvalues, which may be complex, have absolute values that are strictly less than $r_{\mathbf{A}}$ for a positive matrix ($\mathbf{A} > 0$). $r_{\mathbf{A}}$ is the Perron-Frobenius eigenvalue in this instance.

Linear systems. A system of linear equations is produced when different differential equations are subjected to the linear discretization procedure. The discretized differential equation at interior nodes is represented by the first set of equations, while the solution values at boundary points are defined by the remaining equations.These equations can be expressed as follows in matrix-vector notation:

$$\mathbf{L}^h\mathbf{U}^h = \mathbf{F}^h, \tag{3.1}$$

$$\mathbf{U}^h = \begin{pmatrix} \mathbf{u}^i \\ \mathbf{u}^b \end{pmatrix}, \quad \mathbf{F}^h = \begin{pmatrix} \mathbf{f}^i \\ \mathbf{f}^b \end{pmatrix}, \mathbf{L}^h = \begin{pmatrix} \mathbf{A}^i & \mathbf{A}^b \\ \mathbf{O} & \mathbf{I}_m \end{pmatrix} \in \mathbb{R}^{(n+m)\times(n+m)}, \tag{3.2}$$

where $\mathbf{A}^i \in \mathbb{R}^{n\times n}$,$\mathbf{A}^b \in \mathbb{R}^{n\times m}$, $\mathbf{u}^i, \mathbf{f}^i \in \mathbb{R}^n$,$\mathbf{u}^b, \mathbf{f}^b \in \mathbb{R}^m$, $m, n > 0$. From (1), the linear system for the interior nodes can be formulated as follows:

$$\mathbf{A}^i\mathbf{u}^i = \mathbf{f}^i - \mathbf{A}^b\mathbf{f}^b. \tag{3.3}$$

3.1 M-matrices:

The idea of M-matrix was first presented by A. Ostrowski [30] in connection with the research of Herman Minkowski [28]. In this thesis, H. Minkowski established that for a matrix **A** $\in \mathbb{R}^{n\times n}$, given the conditions $a_{ij} < 0$ for $i \neq j$, and the sum $\sum_{j=1}^{n} a_{ij} > 0$ for $i = 1, \ldots, n$, the inequality det(**A**) > 0 is valid. The second condition is known as the strict diagonal dominance condition. Ostrowski employed a less stringent condition $a_{ij} \leq 0$ for $i \neq j$. We shall now define specific classes of matrices and outline their fundamental characteristics.

3.1.0.1 Definition (Z-matrix)**.** A matrix **A** $\in \mathbb{R}^{n\times m}$ is designated as a Z*-matrix* if it fulfills the subsequent criterion: $a_{ij} \leq 0, \quad i \neq j.$

Square Z-matrices are represented by: $Z_n := \{\mathbf{A} \in \mathbb{R}^{n\times n} : a_{ij} \leq 0, i \neq j\}$.

3.1.0.2 Definition (Monotone Matrices)**.** If **A** $\in \mathbb{R}^{n\times n}$ is nonsingular and $\mathbf{A}^{-1} \geq 0$, it is referred to as a monotone matrix.

If two matrices $\mathbf{A}_1$ and $\mathbf{A}_2$ are both monotone, then their product $\mathbf{A}_1\mathbf{A}_2$ is also a monotone matrix. Furthermore, if $\mathbf{A}_1 \leq \mathbf{A}_2$, then their inverses satisfy the inequality: $0 \leq \mathbf{A}_2^{-1} \leq \mathbf{A}_1^{-1}$.

3.1.0.3 Lemma (Equivalent defination of a monotone matrix [2, Lemm 6.1])**.** *A matrix* **A** $\in \mathbb{R}^{n\times n}$ *is monotone if and only if for any vector* **v** $\in \mathbb{R}^n$*, the condition* **Av** ≥ 0 *ensures that* **v** ≥ 0.

3.1.0.4 Corollary. *Consider the monotone matrix* **A** $\in \mathbb{R}^{n\times n}$*. If the inequality* **Av** $\leq$ **Aw** *applies for two vectors* **v**,**w** $\in \mathbb{R}^n$*, then* **v** $\leq$ **w**.

Take into account matrices $\mathbf{A}, \mathbf{M}, \mathbf{N}$ that are part of the space of real $n \times n$ matrices. If the matrix **M** is not singular and the matrix $\mathbf{R} := \mathbf{M}^{-1}\mathbf{N} \geq 0$, then the decomposition $\mathbf{A} = \mathbf{M} - \mathbf{N}$ must be a nonnegative splitting. To be considered a convergent splitting, the nonnegative splitting must meet the condition $\rho(\mathbf{R}) < 1$.

3.1.0.5 Theorem ([2, Theorem 6.16])**.** *The following statements are equivalent if the splitting* $\mathbf{A} = \mathbf{M} - \mathbf{N}$ *is nonnegative and the spectral radius of the matrix* **R** *is provided by* $\rho(\mathbf{R})$.

(i) *A convergent splitting is formed by* $\rho(\mathbf{R}) < 1$*, which indicates that* $\mathbf{A} = \mathbf{M} - \mathbf{N}$.

(ii) $\mathbf{I} - \mathbf{R}$ *is a monotone matrix.*

(iii) **A** *is nonsingular matrix, and we define the matrix* $\mathbf{Q} = \mathbf{A}^{-1}\mathbf{N}$*, which is greater than or equal to zero.*

(iv) **A** *is nonsingular and the spectral radius of* **R** *satisfies:* $\rho(\mathbf{R}) = \rho(\mathbf{Q})/(1 + \rho(\mathbf{Q}))$*, where* $\mathbf{Q} = \mathbf{A}^{-1}\mathbf{N}$.

3.1.0.6 Definition (M-matrices)**.** A matrix **A** $\in \mathbb{R}^{n\times n}$ is designated as a M-matrix if it fulfills the subsequent criteria:

(i) Every off-diagonal elements are non-positive, which means that for $i \neq j$, $a_{ij} \leq 0$.

(ii) Matrix **A** is nonsingular, and its inverse $\mathbf{A}^{-1}$ is non-negative.

3.1.0.7 Definition (Stieltjes matrices)**.** Stieltjes matrices are **A**-matrices that are symmetric and positive definite.

In addition, according to [45, Corollary 3.24]. the irreducibility of Stieltjes matrix **A** is strictly defined as the condition $\mathbf{A}^{-1} > 0$. More than fifty definitions of the M-matrix are equivalent. But we'll narrow our definitional focus to the ones that are most applicable to our issue here in order to do our research.

3.1.0.8 Lemma. *[35, Theorem 2.1] If* **A** *is a matrix in* $\mathbb{Z}_n$ *and* $a_{ii} > 0$ *for all* $i = 1, \ldots, n$*, then the statement "Matrix* **A** *is an M-matrix" can be expressed as any of the following:*

(i) Matrix **A** *has monotone behavior, i.e* $\mathbf{A}^{-1}$ *exists and* $\mathbf{A}^{-1} \geq 0$*.*

(ii) All significant minors of matrix **A** *are nonnegative.*

(iii) $\mathbf{A} = s\mathbf{I} - \mathbf{B}$*, where* **B** *is a nonnegative matrix and* $s > \rho(\mathbf{B})$*;*

(iv) Re $\lambda(\mathbf{A}) > 0$*, where* $\lambda(\mathbf{A})$*is the eigenvalue of the matrix* **A***.*

(v) The vector $\mathbf{v} \in \mathbb{R}^n$*,* $\mathbf{v} > 0$*, such that* $\mathbf{Av} > 0$*, is a (majorizing) vector.*

We are only able to include leading principal minors in statement (ii). $\mathbf{A} + \mathbf{D}$ *is an M-matrix for all nonnegative diagonal matrices* **D** *if* **A** *is a M-matrix.*

3.1.0.9 Example (2x2 M-matrices)**.** A matrix **A** belongs to the set of real numbers and has dimensions of 2×2 *is an* M*-matrix if and only if* $a_{11}, a_{22} > 0$, $a_{12}, a_{21} \leq 0$, det **A** > 0 *(see (ii)). In accordance with (iii), a matrix* $\mathbf{A} = \mathbf{I} - \mathbf{B}$ is an M-matrix is defined by the condition that $\rho(\mathbf{B}) < 1$.

3.1.0.10 Lemma. *Let* $\mathbf{D} \in \mathbb{R}^{2\times 2}$*. If* $\mathbf{D} \geq 0$*,* $|\det \mathbf{D}| < 1$*,* $\operatorname{tr} \mathbf{D} < 1 + \det \mathbf{D}$*, then* $\mathbf{A} = \mathbf{I} - \mathbf{D}$ *is an M-matrix.*

Proof. The characteristic equation $\lambda^2 - \operatorname{tr} \mathbf{D}\lambda + \det \mathbf{D} = 0.$ is satisfied by the eigenvalues of the matrix **D**. If the coefficients of a real polynomial $\lambda^2 + b\lambda + c$ of the second order fulfill the two inequalities $|c| < 1$ and $|b| < c + 1$, then, according to the famous Hurwitz criterion [41], both roots of the polynomial will lie inside the unit circle.It implies that tr $\mathbf{D} > 0$ since $\mathbf{D} \geq 0$. □

3.1.0.11 Corollary. *[2, Lemma 6.2] Consider* $\mathbf{A} \in \mathbb{R}^{n\times n}$ *be a legitimate Minkowski matrix. Then,* **A** *is classified as an M-matrix.*

3.1.0.12 Corollary. *[45, Corollary 3.20],[2, Theorem 4.9] Consider* $\mathbf{A} \in \mathbb{R}^{n\times n}$ *as an irreducibly diagonally dominant Minkowski matrix, where* $a_{ii} > 0$ *for each* $i = 1, \ldots, n$*. Consequently,* **A** *qualifies as a* M*-matrix, and it follows that* $\mathbf{A}^{-1} > 0$*.*

Let us consider a two-by-two block matrix

$$\mathbf{M} = \begin{pmatrix} \mathbf{E} & \mathbf{F} \\ \mathbf{G} & \mathbf{H} \end{pmatrix}, \tag{3.4}$$

where

$$\mathbf{E} \in \mathbb{R}^{n\times n}, \mathbf{F} \in \mathbb{R}^{n\times m}, \mathbf{G} \in \mathbb{R}^{m\times n}, \mathbf{H} \in \mathbb{R}^{m\times m}, \quad 0 < n, m,$$

if the block matrices satisfy $\mathbf{F} \leq 0$, $\mathbf{G} \leq 0$ and if **H** is nonsingular, then the Schur complement of **H** in **M** is given by:

$$\mathbf{S} = \mathbf{E} - \mathbf{F}\mathbf{H}^{-1}\mathbf{G}$$

According to [28], If **M** is an M matrix, then both the matrices **E** and **H** are M-matrices.
From the decomposition of matrix **M**,

$$\begin{pmatrix} \mathbf{E} & \mathbf{F} \\ \mathbf{G} & \mathbf{H} \end{pmatrix} = \begin{pmatrix} \mathbf{I}_n & \mathbf{F}\mathbf{H}^{-1} \\ \mathbf{O} & \mathbf{I}_m \end{pmatrix} \begin{pmatrix} \mathbf{S} & \mathbf{O} \\ \mathbf{O} & \mathbf{H} \end{pmatrix} \begin{pmatrix} \mathbf{I}_n & \mathbf{O} \\ \mathbf{H}^{-1}\mathbf{G} & \mathbf{I}_m \end{pmatrix}$$

we obtain the inverse:

$$\mathbf{M}^{-1} = \begin{pmatrix} \mathbf{I}_n & \mathbf{O} \\ -\mathbf{H}^{-1}\mathbf{G} & \mathbf{I}_m \end{pmatrix} \begin{pmatrix} \mathbf{S}^{-1} & \mathbf{O} \\ \mathbf{O} & \mathbf{H}^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{I}_n & -\mathbf{F}\mathbf{H}^{-1} \\ \mathbf{O} & \mathbf{I}_m \end{pmatrix}$$

$$= \begin{pmatrix} \mathbf{S}^{-1} & -\mathbf{S}^{-1}\mathbf{F}\mathbf{H}^{-1} \\ -\mathbf{H}^{-1}\mathbf{G}\mathbf{S}^{-1} & \mathbf{H}^{-1} + \mathbf{H}^{-1}\mathbf{G}\mathbf{S}^{-1}\mathbf{F}\mathbf{H}^{-1} \end{pmatrix}$$

It follows that if **M** is a M-matrix, then **S** is also a M-matrix. If $\mathbf{G} = 0$, it follows that **M** is classified as a reducible matrix. In this scenario, **M** qualifies as a M-matrix if and only if both **E** and **H** are classified as M-matrices. If, $\mathbf{H} = \mathbf{I}$, then **M** takes on the structure outlined in (2).

3.1.0.13 Definition (Elliptic Partial Differential Equations in 2D)**.** A second-order linear PDE in two dimensions has the general form:

$$Lu = -\left(a(x,y)\frac{\partial^2 u}{\partial x^2} + 2b(x,y)\frac{\partial^2 u}{\partial x \partial y} + c(x,y)\frac{\partial^2 u}{\partial y^2} \right) + (\text{lower order terms}) = f(x,y)$$

The equation is said to be elliptic at a point (x, y) if the discriminant condition holds:

$$ac - b^2 > 0$$

The most common elliptic PDE is the Poisson equation:

$$-\Delta u = f(x,y),\ in\, \Omega \subset R^2$$

3.1.0.14 Definition (Local boundary conditios)**.** Local boundary conditions apply pointwise on the domain boundary $\partial\Omega$:

1. Dirichlet Condition: $u(x, y) = g(x, y), \quad (x, y) \in \partial\Omega$
2. Neumann Condition:

$$\frac{\partial u}{\partial n}(x, y) = h(x, y)$$

3. Robin Condition:

$$\alpha u + \beta \frac{\partial u}{\partial n} = r(x, y)$$

3.1.0.15 Definition (Nonlocal Boundary Conditions)**.** Nonlocal boundary conditions (NBCs) involve integral relations over the boundary or entire domain. For example:

1. Boundary Integral Condition:

$$u(x, y) = \int_{\partial\Omega} K((x, y), (s, t))u(s, t)ds\, dt$$

2. Domain Integral Condition:

$$\frac{\partial u}{\partial n}(x, y) = \int_{\Omega} \rho((x, y), (\xi, \eta))u(\xi, \eta)d\xi\, d\eta$$

These conditions are useful in modeling long-range interactions and arise naturally in fractional diffusion, population dynamics, and materials with memory.

3.2 Chebyshev polynomials

3.2.0.1 Definition (Chebyshev polynomials)**.** The Chebyshev polynomials consist of two sequences of polynomial functions, indicated by $P_n(z)$ and $Q_n(z)$, which are intimately connected with trigonometric functions, especially sine and cosine. These polynomials can be defined through various equivalent approaches, one of which involves trigonometric identities. The Chebyshev polynomials of the first kind, represented by P_n, are defined as $P_n(\cos\phi) = \cos(n\phi)$. Similarly, the Chebyshev polynomials of the second kind denoted by Q_n, are given by $Q_n(\cos\phi)\sin\phi = \sin((n+1)\phi)$. At first glance, these expressions may not appear to be polynomial functions in $\cos\phi$, but this becomes evident by applying trigonometric identities such as de Moivre's formula or the angle addition formulas repeatedly.

For instance, using the double-angle identities:

$$P_2(\cos\phi) = \cos(2\phi) = 2\cos^2\phi - 1$$

$$Q_1(\cos\phi)\sin\phi = \sin(2\phi) = 2\cos\phi\sin\phi$$

These demonstrate that:

$$P_2(z) = 2z^2 - 1, \quad \text{and} \quad Q_1(z) = 2z$$

confirming that they are indeed polynomials in $z = \cos\phi$.

A key and useful characteristic of the Chebyshev polynomials $P_n(z)$ is their orthogonality under a specific inner product, defined as

$$\langle f, g\rangle = \int_{-1}^{1} \frac{f(z)\,g(z)}{\sqrt{1-z^2}}\,dz$$

In contrast, the polynomials $Q_n(z)$ are orthogonal with respect to a different, but similar, inner product. The Chebyshev polynomials P_n also have the notable property of having the greatest possible leading coefficient among all polynomials that remain within the range of $[-1,1]$ on the interval $[-1,1]$. This makes them "extremal" polynomials in various contexts.

3.2.0.2 Definition (Recurrence definition)**.** The Chebyshev polynomials of the first kind can be defined recursively using the relation $P_0(z) = 1, \quad P_1(z) = z, \quad P_{n+1}(z) = 2zP_n(z) - P_{n-1}(z)$. This recurrence also makes it possible to express $P_k(z)$ as the determinant of a tridiagonal matrix of size $k \times k$:

$$P_k(z) = \det \begin{bmatrix} 2z & -1 & 0 & \cdots & 0 \\ -1 & 2z & -1 & \ddots & \vdots \\ 0 & -1 & 2z & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & 0 & -1 & 2z \end{bmatrix}$$

Additionally, the ordinary generating function for $P_n(z)$ is given by:

$$\sum_{n=0}^{\infty} P_n(z)t^n = \frac{1-tz}{1-2tz+t^2}$$

Beyond the standard generating function, there are several other forms related to Chebyshev polynomials. The exponential generating function is given by:

$$\sum_{n=0}^{\infty} \frac{P_n(z)t^n}{n!} = \frac{1}{2}\left(e^{t(z-\sqrt{z^2-1})} + e^{t(z+\sqrt{z^2-1})}\right) = e^{tz}\,\text{cosh}\left(t\sqrt{z^2-1}\right)$$

Another important generating function, particularly useful in two-dimensional potential theory and multipole expansions, is:

$$\sum_{n=1}^{\infty} \frac{P_n(z)t^n}{n} = \text{ln}\left(\frac{1}{\sqrt{1-2tz+t^2}}\right)$$

The second-kind Chebyshev polynomials, represented by $Q_n(z)$, obey the recurrence relation.:

$$Q_0(z) = 1, \quad Q_1(z) = 2z, \quad Q_{n+1}(z) = 2z\,Q_n(z) - Q_{n-1}(z)$$

This relation is almost identical to that of the first kind, except that $P_1(z) = z$ while $Q_1(z) = 2z$.

For $Q_n(z)$, the standard generating function is:

$$\sum_{n=0}^{\infty} Q_n(z)\,t^n = \frac{1}{1-2tz+t^2}$$

The generating function for exponential growth is provided by:

$$\sum_{n=0}^{\infty} \frac{Q_n(z)\,t^n}{n!} = e^{tz}\left(\text{cosh}\left(t\sqrt{z^2-1}\right) + \frac{z}{\sqrt{z^2-1}}\,\text{sinh}\left(t\sqrt{z^2-1}\right)\right)$$

3.3 Kronecker Product

3.3.0.1 Definition. (Kronecker Product) Let X be an $r \times s$ matrix, and Y be a $t \times u$ matrix. Then the Kronecker product $X \otimes Y$ is defined as the $(rt) \times (su)$ block matrix:

$$\mathbf{X} \otimes \mathbf{Y} = \begin{bmatrix} x_{11}\mathbf{Y} & x_{12}\mathbf{Y} & \cdots & x_{1s}\mathbf{Y} \\ x_{21}\mathbf{Y} & x_{22}\mathbf{Y} & \cdots & x_{2s}\mathbf{Y} \\ \vdots & \vdots & \ddots & \vdots \\ x_{r1}\mathbf{Y} & x_{r2}\mathbf{Y} & \cdots & x_{rs}\mathbf{Y} \end{bmatrix} \in \mathbb{R}^{rt \times su}$$

Fundamental Properties of the Kronecker Product:

1. **Associative Property:**
$$(\mathbf{L} \otimes \mathbf{M}) \otimes \mathbf{N} = \mathbf{L} \otimes (\mathbf{M} \otimes \mathbf{N})$$

2. **Product Rule:**
$$(\mathbf{L} \otimes \mathbf{M})(\mathbf{N} \otimes \mathbf{S}) = (\mathbf{LN}) \otimes (\mathbf{MS}) \quad \text{(if dimensions are compatible)}$$

3. **Transpose and Conjugate Transpose:**
$$(\mathbf{L} \otimes \mathbf{M})^T = \mathbf{L}^T \otimes \mathbf{M}^T$$
$$(\mathbf{L} \otimes \mathbf{M})^* = \mathbf{L}^* \otimes \mathbf{M}^*$$

4. **Inverse of Kronecker Product:**
$$(\mathbf{L} \otimes \mathbf{M})^{-1} = \mathbf{L}^{-1} \otimes \mathbf{M}^{-1} \quad \text{(if } \mathbf{L} \text{ and } \mathbf{M} \text{ are invertible)}$$

5. **Trace and Determinant:**
$$\text{tr}(\mathbf{L} \otimes \mathbf{M}) = \text{tr}(\mathbf{L}) \cdot \text{tr}(\mathbf{M})$$
$$\det(\mathbf{L} \otimes \mathbf{M}) = \det(\mathbf{L})^t \cdot \det(\mathbf{M})^r \quad \text{(for } \mathbf{L} \in \mathbb{R}^{r \times r}, \mathbf{M} \in \mathbb{R}^{t \times t}\text{)}$$

6. **Eigenvalues and Eigenvectors:**
   - If α_i are eigenvalues of **L** and β_j are eigenvalues of **M**, then $\alpha_i\beta_j$ are eigenvalues of $\mathbf{L} \otimes \mathbf{M}$
   - The associated eigenvectors are $\mathbf{l}_i \otimes \mathbf{m}_j$, where $\mathbf{l}_i$ and $\mathbf{m}_j$ are eigenvectors of **L** and **M**, respectively

7. **Kronecker Sum (for Square Matrices):**
$$\mathbf{L} \oplus \mathbf{M} = \mathbf{L} \otimes \mathbf{I}_t + \mathbf{I}_r \otimes \mathbf{M} \quad \text{(where } \mathbf{L} \in \mathbb{R}^{r \times r}, \mathbf{M} \in \mathbb{R}^{t \times t}\text{)}$$

Chapter 4

Discretization of elliptic equations using finite differences with nonlocal boundary terms

The finite-difference method (FDM) is employed to approximate solutions of elliptic boundary value problems. Consider the rectangular domain defined as $\Omega = [0,p] \times [0,q]$. A uniform grid ω^k is defined with steps $k_x = p/S$ and $k_y = q/T$, where $S, T \in \mathbb{N}$ and $0 < S, T$. Let k^2 be defined as $k_x k_y$. The grid is characterized as follows:

$$\overline{\omega}_x^k = \{x_r : x_r = r.k_x,\, r \in \overline{I}_x\}, \quad \overline{I}_x = \{r : r = 0, \ldots, S\}$$

$$\overline{\omega}_y^k = \{y_s : y_s = s.k_y,\, s \in \overline{I}_y\}, \quad \overline{I}_y = \{s : s = 0, \ldots, T\}$$

$$\Omega^k = \overline{\omega}^k = \overline{\omega}_x^k \times \overline{\omega}_y^k = \{x_{rs} = (x_r, y_s) : (r,s) \in \overline{I}\}, \quad \overline{I} = \overline{I}_x \times \overline{I}_y$$

We will denote the grid functions $U : \omega^k \to \mathbb{R}$ as $U_{rs} = U(x_{rs})$.
We list $K = (S+1)(T+1)$ grid $\overline{\omega}^k$ nodes.

$$x_{00} < \ldots < x_{0S} < x_{01} < \ldots < x_{S1} < \ldots < x_{ST},$$

i.e., we can use vector of nodes $(\bar{x}_1, \ldots, \bar{x}_K) =$ vec$(x_{rs} : (r,s) \in \overline{\mathcal{I}})$ numbered with a single index.

Grid $\overline{\omega}^k = \overline{\omega}_x^k$, $\overline{\mathcal{I}} = \overline{\mathcal{I}}_x$, $k = k_x$ will be used for one-dimensional problems in $\Omega = [0,p]$. The natural order of the nodes is $x_0 < x_1 < \ldots < x_S$, $(\bar{x}_1, \ldots, \bar{x}_{S+1})$= $(x_0, \ldots, x_S)$. One-dimensional grid is two-dimensional grid in the case $0 < S, T = 0$, $\overline{\mathcal{I}}_y = \{0\}$. In this case $x_r = x_{r0}$, $r = 0, \ldots, S$ and $U_r = U_{r0}$, $r \in \overline{\mathcal{I}}$, for grid functions. We will use spatial variable $u \in [0,p]$ for Sturm–Liouville Problems and one-dimensional grid $\omega_u^k := \{u_r : u_r = r \cdot k, r \in \overline{\mathcal{I}}_u = \overline{\mathcal{I}}_x\}$, $k = p/S$.
We will list the subgrid nodes in the same order as in $\overline{\omega}^k$ if subgrid $\omega \subset \overline{\omega}^k$. However, we will skip the nodes that don't belong to ω: $(\bar{x}_1, \ldots, \bar{x}_k) =$ vec$_\omega(x_{rs} : x_{rs} \in \omega)$, where $k = |\omega|$ is the number of nodes in the ω subgrid.

The subgrids for inner and boundary nodes in this thesis are denoted by ω, $\partial\omega$, and $\overline{\omega}$, respectively. Please take note that $\overline{\omega}$ might not equal $\overline{\omega}^k$. The two-dimensional subgrid $\overline{\omega} = \widetilde{\omega}^k \neq \overline{\omega}^k$, where inner nodes are $\omega = \omega^k$, boundary nodes are $\partial\omega = \partial\omega^k$, and

$$\begin{aligned}
&\omega_x^k := \{x_r : x_r = r \cdot k_x, r \in \mathcal{I}_x\}, \quad \mathcal{I}_x := \{r : r = 1, \dots, S-1\};\\
&\omega_y^k := \{y_s : y_s = s \cdot k_y, s \in \mathcal{I}_y\}, \quad \mathcal{I}_y := \{s : s = 1, \dots, T-1\};\\
&\omega^k = \omega_x^k \times \omega_y^k = \{x_{rs} = (x_r, y_s) : (r,s) \in \mathcal{I}\}, \quad \mathcal{I} := \mathcal{I}_x \times \mathcal{I}_y;\\
&\widetilde{\omega}^k = \overline{\omega}^k \setminus \{x_{00}, x_{S0}, x_{0T}, x_{ST}\}; \quad \partial\omega^k := \widetilde{\omega}^k \setminus \overline{\omega}^k
\end{aligned}$$

When two disjoint linearly ordered sets are added together, the notation $\overline{\omega} = \omega + \partial\omega$ is used.

Regarding grid functionalities, The vector $\mathbf{U} = (\mathbf{U}^i, \mathbf{U}^b)^T$ is constructed using $U : \overline{\omega} \to \mathbb{R}$:

$$\mathbf{U}^i := (U_1^i, \dots, U_n^i)^T := \mathrm{vec}(U_{rs} : x_{rs} \in \omega), \quad n = |\omega|;$$

$$\mathbf{U}^b := (U_1^b, \dots, U_m^b)^T := \mathrm{vec}(U_{rs} : x_{rs} \in \partial\omega), \quad m = |\partial\omega|.$$

For the grid functions $U : \omega^k \to \mathbb{R}$ ($U : \omega_x^k \to \mathbb{R}$), we will make use of the grid operators δ_x^2 and δ_y^2. In the case of the one-dimensional scenario, δ^2 = δ_x^2.

$$\delta_x^2 U_{rs} = \frac{U_{r-1,s} - 2U_{rs} + U_{r+1,s}}{k_x^2}, \quad \delta_y^2 U_{rs} = \frac{U_{r,s-1} - 2U_{rs} + U_{r,s+1}}{k_y^2}, \quad x_{rs} \in \omega^k.$$

We will now show and briefly discuss a relatively basic example illustrating the function of *M*-matrices in solving boundary value issues for elliptic equations via the finite-difference approach. Take into account the differential problem:

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = f(x,y), \quad (x,y) \in \Omega, \tag{3.1}$$

,

$$u|_{\partial\Omega} = g(x,y), \quad (x,y) \in \partial\Omega, \tag{3.2}$$

,

and the corresponding FDS on the grid $\widetilde{\omega}^k = \omega + \partial\omega$, $\omega = \omega^k \times \omega^k$, $\partial\omega = \partial\omega^k$:

$$-\delta_x^2 U_{rs} - \delta_y^2 U_{rs} = F_{rs}, \quad x_{rs} \in \omega, \tag{3.3}$$

$$U_{r0} = G_{r0}, \quad U_{rS} = G_{rS}, \quad x_r \in \omega_x^k, \quad U_{0s} = G_{0s}, \quad U_{Ss} = G_{Ss}, \quad y_s \in \omega_y^k. \tag{3.4}$$

FDS (3.3)–(3.4) can be expressed as (2.1)–(2.2).

$$\mathbf{L}^h \mathbf{U}^h = \mathbf{F}^h, \quad \mathbf{U}^h = \begin{pmatrix} \mathbf{U}^i \\ \mathbf{U}^b \end{pmatrix}, \quad \mathbf{F}^h = \begin{pmatrix} \mathbf{F}^i \\ \mathbf{F}^b \end{pmatrix},$$

$$\mathbf{L}^h = \begin{pmatrix} \mathbf{A}^i & \mathbf{A}^b \\ \mathbf{O} & \mathbf{I}_m \end{pmatrix} \in \mathbb{R}^{(n+m)\times(n+m)},$$

where $n = |\omega^k| = (S-1)(T-1)$, $m = |\partial\omega^k| = 2(S+T)-4$, $\mathbf{A}^i \in \mathbb{R}^{n\times n}$, $\mathbf{A}^b \in \mathbb{R}^{n\times m}$, $\mathbf{U}^i, \mathbf{F}^i = \text{vec}(F_{rs} : x_{rs} \in \omega) \in \mathbb{R}^n$, $\mathbf{U}^b, \mathbf{F}^b = \text{vec}(G_{rs} : x_{rs} \in \partial\omega) \in \mathbb{R}^m$.

$\mathbf{A}^i$ is a block tridiagonal matrix for the FDS (3.3)–(3.4) .

$$\mathbf{A}^i = \begin{pmatrix} A_0 & -k_y^{-2}I & & \\ -k_y^{-2}I & A_0 & \ddots & \\ & \ddots & \ddots & -k_y^{-2}I \\ & & -k_y^{-2}I & A_0 \end{pmatrix}, \tag{3.5}$$

where the identity matrix is $\mathbf{I} \in \mathbb{R}^{(S-1)\times(S-1)}$ and $\mathbf{A}_0 \in \mathbb{R}^{(S-1)\times(S-1)}$,

$$\mathbf{A}_0 = \begin{pmatrix} 2k_x^{-2}+2k_y^{-2} & -k_x^{-2} & & \\ -k_x^{-2} & 2k_x^{-2}+2k_y^{-2} & \ddots & \\ & \ddots & \ddots & -k_x^{-2} \\ & & -k_x^{-2} & 2k_x^{-2}+2k_y^{-2} \end{pmatrix}$$

$$\mathbf{A}^b = \begin{pmatrix} -k_y^{-2}\mathbf{I} & -k_x^{-2}\mathbf{J} & & & \\ & & -k_x^{-2}\mathbf{J} & & \\ & & & \ddots & \\ & & & & -k_x^{-2}\mathbf{J} \quad -k_y^{-2}\mathbf{I} \end{pmatrix}, \quad \mathbf{J} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \\ 0 & 1 \end{pmatrix} \in \mathbb{R}^{(S-1)\times 2}$$

,

For inner nodes (2.3), the linear system can be expressed as

$$\mathbf{A}^i\mathbf{U}^i = \mathbf{F}, \quad \mathbf{F} = \mathbf{F}^i - \mathbf{A}^b\mathbf{F}^b, \tag{3.6}$$

where $\mathbf{F} \in \mathbb{R}^n$, $\mathbf{A}^i \in \mathbb{R}^{n\times n}$.

Let us enumerate the essential characteristics of matrix $\mathbf{A}^i$.:

1. Matrix $\mathbf{A}^i$ is characterized as a block tridiagonal irreducible matrix.;
2. The Matrix $\mathbf{A}^i$ is symmetric and positively defined.
3. The diagonal elements $a_{jj} = 2k_x^{-2} + 2k_y^{-2}$ of matrix $\mathbf{A}^i$ are positive.;
4. non-diagonal elements $(j, l = 1, \dots, n,\ j \neq l)$ of matrix $\mathbf{A}^i$ are non-positive, $a_{jl} = -k_x^{-2}$, or $a_{jl} = -k_y^{-2}$, or $a_{jl} = 0$;
5. all eigenvalues of $\mathbf{A}^i$ are positive:

$$\lambda_{rs} = 4\left(k_x^{-2}\sin^2\left(\frac{\pi}{2}k_x r\right) + k_y^{-2}\sin^2\left(\frac{\pi}{2}k_y s\right)\right), \quad r = 1, \dots, S-1,\ s = 1, \dots, T-1;$$

6. As the basis of the vector space $\mathbb{R}^n$, the collection of eigenvectors of matrix $\mathbf{A}^i$ is orthonormal.

The above properties of matrix $\mathbf{A}^i$ provide sufficient information to draw the following conclusion: $\mathbf{A}^i$ qualifies as a M-matrix, specifically a Stieltjes matrix. It is important to note that the matrix $\mathbf{L}^h$ is also classified as a M-matrix.

In order to finalize the methodological discussion, we revisit the issue outlined in (3.1)–(3.2), substituting the boundary condition $u|_{\partial\Omega} = g$ at one side of the rectangle Ω with a nonlocal condition. Specifically, we replace condition (3.2) with the following:

$$u(x,0) = g_1(x), \quad u(x,1) = g_3(x), \quad x \in [0,1], \quad u(1,y) = g_2(y), \quad y \in [0,1], \tag{3.7}$$

$$u(0,y) = \gamma \int_0^1 u(x,y)\,dx + g_4(y), \quad y \in (0,1), \tag{3.8}$$

where $\gamma > 0$ represents a specified constant. When $\gamma = 0$, the problem defined by equations (3.1) and (3.8)–(3.7) aligns with the problem represented by equations (3.1)–(3.2). The integral condition (3.8) is representative of the current research focus on problems involving nonlocal conditions [4][7][9].

Condition (3.8) is approximated using the trapezoid rule

$$U_{0s} = \gamma k_x \left(\frac{U_{0s}}{2} + \sum_{r=1}^{S-1} U_{rs} + \frac{U_{Ss}}{2} \right) + G_{0s}, \quad y_s \in \omega_y^k, \tag{3.9}$$

we obtain problem (3.3), (3.9) and

$$U_{r0} = G_{r0}, \quad U_{rS} = G_{rS}, \quad x_r \in \omega_x^k, \quad U_{Ss} = G_{Ss}, \quad y_s \in \omega_y^k, \tag{3.10}$$

In place of the earlier difference problem (3.3)–(3.4). We will utilize three types of block matrices $\mathbf{B^i}, \mathbf{B^n} \in \mathbb{R}^{m\times n}$ and $\mathbf{B}^b \in \mathbb{R}^{m\times n}$ to describe the boundary conditions (3.9)–(3.10):

$$\mathbf{B}^k = \begin{pmatrix} \mathbf{B}_0^k & & & \\ \mathbf{B}_1^k & & & \\ & \ddots & & \\ & & \mathbf{B}_{S-1}^k & \\ & & \mathbf{B}_S^k & \end{pmatrix}, \quad \mathbf{B}^b = \begin{pmatrix} \mathbf{B}_0^b & & & & \\ & \mathbf{B}_1^b & & & \\ & & \ddots & & \\ & & & \mathbf{B}_{S-1}^b & \\ & & & & \mathbf{B}_S^b \end{pmatrix},$$

in such case $k = r, n$. Our next step is to convert these boundary conditions to a matrix form:

$$\mathbf{U}^b = \mathbf{B}^b\mathbf{U}^b + \mathbf{B}^i\mathbf{U}^i + \mathbf{F}^b, \quad \mathbf{B}^b \geq 0, \mathbf{B}^i \geq 0, \tag{3.11}$$

where $\mathbf{B}_0^b = \mathbf{B}_S^b = \mathbf{B}_0^i = \mathbf{B}_S^i = \mathbf{O} \in \mathbb{R}^{(S-1)\times(S-1)}$, $(\mathbf{I} - \mathbf{B}_s^b)^{-1} = (\mathbf{I} - \mathbf{B}_S^b)^{-1} = \mathbf{I}$,

$$\mathbf{B}_s^b = \begin{pmatrix} \gamma k_x/2 & \gamma k_x/2 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{B}_s^i = \begin{pmatrix} \gamma k_x & \cdots & \gamma k_x \\ 0 & \cdots & 0 \end{pmatrix} \in \mathbb{R}^{2\times(S-1)},$$

$$(\mathbf{I} - \mathbf{B}_s^b)^{-1} = \frac{1}{1-\gamma k_x/2}\begin{pmatrix} 1 & \gamma k_x/2 \\ 0 & 1-\gamma k_x/2 \end{pmatrix}, \quad s = 1, \dots, S-1.$$

Problem (3.3) and equations (3.11)–(3.12) can be reformulated as:

$$\mathbf{A}^i\mathbf{U}^i + \mathbf{A}^b\mathbf{U}^b = \mathbf{F}^i, \tag{3.12}$$

$$\mathbf{A}^{bi}\mathbf{U}^i + \mathbf{A}^{bb}\mathbf{U}^b = \mathbf{F}^b, \tag{3.13}$$

and we have the block matrix

$$\mathbf{L}^h := \begin{pmatrix} \mathbf{A}^i & \mathbf{A}^b \\ \mathbf{A}^{bi} & \mathbf{A}^{bb} \end{pmatrix}, \quad \mathbf{A}^b \le 0, \mathbf{A}^{bi} = -\mathbf{B}^i \le 0, \mathbf{A}^{bb} = \mathbf{I} - \mathbf{B}^b, \tag{3.14}$$

of the form (2.4), $\mathbf{A}^i$ is an M-matrix.

The next lemma is true based on block matrix properties (2.4).

4.0.0.1 Lemma. *Let* $\mathbf{L}^h$ *be given with the block structure (3.14). If* $\mathbf{L}^h$ *is an* M*-matrix then* $\mathbf{A}^i, \mathbf{A}^{bb}$ *and the Schur complement* $\mathbf{S} = \mathbf{A}^i - \mathbf{A}^b(\mathbf{A}^{bb})^{-1}\mathbf{A}^{bi}$ *of the block* $\mathbf{A}^{bb}$ *of the matrix* $\mathbf{L}^h$ *are* M*-matrices.*

It is essential to identify the conditions under which $\mathbf{S}$ qualifies as a M-matrix, noting that $\mathbf{L}^h$ may not necessarily meet the criteria of a M-matrix in this scenario.

Equation (3.13), if $\mathbf{A}^{bb}$ is a M-matrix, is equal to

$$\mathbf{A}^n\mathbf{U}^i + \mathbf{U}^b = \widetilde{\mathbf{F}}^{\mathbf{i}}, \quad \mathbf{A}^n = (\mathbf{A}^{bb})^{-1}\mathbf{A}^{bi} \le 0, \quad \widetilde{\mathbf{F}}^{\mathbf{b}} = (\mathbf{A}^{bb})^{-1}\mathbf{F}^b. \tag{3.15}$$

For boundary conditions (3.11)–(3.12) [19]: $\mathbf{A}^{bb}$ is an M-matrix when $0 \le \gamma k_x < 2$, $\mathbf{A}^n = -\mathbf{B}^n$, where

$$\mathbf{B}_s^n = \begin{pmatrix} \gamma & \cdots & \gamma \\ 0 & \cdots & 0 \end{pmatrix} \in \mathbb{R}^{2\times(S-1)}, \quad s = 1, \dots, S-1, \quad \tilde{\gamma} = \frac{\gamma k_x}{1 - \frac{\gamma k_x}{2}} > 0.$$

For inner nodes, the equation is

$$\mathbf{A}\mathbf{U}^i = \mathbf{F} := \mathbf{F}^i - \mathbf{A}^b\widetilde{\mathbf{F}}^{\mathbf{b}}, \quad \widetilde{\mathbf{F}}^{\mathbf{b}} = (\mathbf{A}^{bb})^{-1}\mathbf{F}^b. \tag{3.16}$$

We have regular splitting $\mathbf{A} = \mathbf{A}^i - \mathbf{C}$, where $\mathbf{C} = \mathbf{A}^b(\mathbf{A}^{bb})^{-1}\mathbf{A}^{bi} \ge 0$. From the system (3.16), we may determine vector $\mathbf{U}^i$, if $\mathbf{A}$ is nonsingular (for example, $\mathbf{A}$, is a M-matrix). Then employing formula (3.15) we obtain

$$\mathbf{U}^b = \widetilde{\mathbf{F}}^b - \mathbf{A}^n\mathbf{U}^i, \quad \mathbf{A}^n := (\mathbf{A}^{bb})^{-1}\mathbf{A}^{bi}.$$

4.0.0.2 Remark. If $\mathbf{A}^{bi} = \mathbf{O}$ and $\mathbf{A}^{bb} = \mathbf{I}$, then $\mathbf{C} = \mathbf{O}$. In this case linear equation (3.16) becomes (3.6).

In the case problem (3.3), (3.9)–(3.10) matrix

$$\mathbf{C} = \text{diag}(E, \dots, E), \tag{3.21}$$

where

$$\mathbf{E} = k_x^{-2}\begin{pmatrix} \tilde{\gamma} & \tilde{\gamma} & \cdots & \tilde{\gamma} \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix} \in \mathbb{R}^{(S-1)\times(S-1)}.$$

For the finite-difference problem (3.3), (3.9)–(3.10), matrix **A** will have the same structure as matrix $\mathbf{A}^i$ (see (3.5)), but matrix $\mathbf{A}_0$ needs to be substituted with $\mathbf{A}_\gamma = \mathbf{A}_0 - \mathbf{E}$ [19], [38]:

$$\mathbf{A}^i = \begin{pmatrix} \mathbf{A}_\gamma & -k_y^{-2}\mathbf{I} & & \\ -k_y^{-2}\mathbf{I} & \mathbf{A}_\gamma & \ddots & \\ & \ddots & \ddots & -k_y^{-2}\mathbf{I} \\ & & -k_y^{-2}\mathbf{I} & \mathbf{A}_\gamma \end{pmatrix},$$

$$\mathbf{A}_\gamma = \begin{pmatrix} (2-\tilde{\gamma})k_x^{-2} + 2k_y^{-2} & -(1+\tilde{\gamma})k_x^{-2} & -\tilde{\gamma}k_x^{-2} & \cdots & -\tilde{\gamma}k_x^{-2} \\ -k_x^{-2} & 2k_x^{-2} + 2k_y^{-2} & -k_x^{-2} & \cdots & \\ & \ddots & \ddots & \ddots & \\ & & -k_x^{-2} & 2k_x^{-2} + 2k_y^{-2} & -k_x^{-2} \\ & & & -k_x^{-2} & 2k_x^{-2} + 2k_y^{-2} \end{pmatrix}$$

For the classical boundary conditions, we have $\mathbf{A}_\gamma = \mathbf{A}_0$, $\mathbf{C} = 0$, and $\mathbf{A} = \mathbf{A}^i$.

The reconfiguration of systems (3.3) and (3.9)–(3.10) indicates that analyzing this system with the nonlocal condition (3.9) necessitates just the examination of systems (3.10)–(3.13) under the Dirichlet condition.

In the event that $0 \le \tilde{\gamma} \le 1 + \frac{2}{2S-1}$, hence $0 \le \tilde{\gamma} < (S-1)^{-1}$. Therefore, the matrix **A** has nondiagonal entries that are nonpositive and diagonal elements that are positive. The structure of $\mathbf{A}_\gamma$ indicates that there is a row with a positive sum and that the sum of the entries in any row of the matrix **A** is nonnegative. For instance, the total of the entries in the final row is positive, and the line with the nonlocal parameter $\tilde{\gamma} \le (S-1)^{-1}$ of the matrix **A** is a nonnegative. The irreducible nature of matrix $\mathbf{A}^i$ makes it an irreducible diagonally dominant Minkowski matrix with positive diagonal members. As a result of Corollary 3, **A** is a M-matrix. As a result, the following assertion holds true for problems (3.3), (3.9), and (3.10).

Chapter 5

Analytical Part

5.1 Generalized Finite Difference Solution for the 2D Poisson Equation

5.1.1 Problem Statement:

Consider the 2D Poisson equation on a rectangular domain $\Omega = (0, l_x) \times (0, l_y)$:

$$-\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = f(x,y), \quad (x,y) \in \Omega,$$

with Dirichlet boundary conditions:

$$u(x,y) = g(x,y) \quad \text{on} \quad \partial\Omega.$$

2. Domain Discretization:

- Grid spacing: $h_x = \frac{l_x}{N_x}, \quad h_y = \frac{l_y}{N_y}$, where N_x and N_y are the number of intervals in x and y directions, respectively.
- Grid points: $x_i = ih_x$ ($i = 0, \ldots, N_x$), $y_j = jh_y$ ($j = 0, \ldots, N_y$).
- Interior points: Total unknowns: $(N_x - 1) \times (N_y - 1)$.

3. Finite Difference Approximation: The second derivatives are approximated using central differences:

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h_x^2},$$

$$\frac{\partial^2 u}{\partial y^2} \approx \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{h_y^2}.$$

Substituting into the Poisson equation:

$$-\left(\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h_x^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{h_y^2}\right) = f_{i,j}.$$

4. Discrete Equation: Combine terms to form the 5-point stencil:

$$-\frac{u_{i+1,j}}{h_x^2} - \frac{u_{i-1,j}}{h_x^2} - \frac{u_{i,j+1}}{h_y^2} - \frac{u_{i,j-1}}{h_y^2} + \left(\frac{2}{h_x^2} + \frac{2}{h_y^2}\right) u_{i,j} = f_{i,j}.$$

Let $\alpha = \frac{1}{h_x^2}$ and $\beta = \frac{1}{h_y^2}$, then:

$$-\alpha(u_{i+1,j} + u_{i-1,j}) - \beta(u_{i,j+1} + u_{i,j-1}) + 2(\alpha + \beta)u_{i,j} = f_{i,j}.$$

5. System Matrix A: The linear system **AU** $=$ **F** is constructed as follows:

a. Unknown Ordering: Use lexicographic (row-wise) ordering for the unknowns $u_{i,j}$:

$$\mathbf{U} = \begin{pmatrix} u_{1,1}, & \dots, & u_{N_x-1,1}, \\ u_{1,2}, & \dots, & u_{N_x-1,2}, \\ \vdots & \ddots & \vdots \\ u_{1,N_y-1}, & \dots, & u_{N_x-1,N_y-1} \end{pmatrix}^T \in \mathbb{R}^{(N_x-1)(N_y-1)}.$$

b. Matrix Structure: The matrix A is block-tridiagonal:

$$\mathbf{A} = \begin{pmatrix} \mathbf{A}_0 & -\beta\mathbf{I} & & 0 \\ -\beta\mathbf{I} & \mathbf{A}_0 & \ddots & \\ & \ddots & \ddots & -\beta\mathbf{I} \\ 0 & & -\beta\mathbf{I} & \mathbf{A}_0 \end{pmatrix},$$

where:

- Each block $\mathbf{A}_0 \in \mathbb{R}^{(N_x-1)\times(N_x-1)}$ is tridiagonal:

$$\mathbf{A}_0 = \begin{pmatrix} 2(\alpha+\beta) & -\alpha & & 0 \\ -\alpha & 2(\alpha+\beta) & \ddots & \\ & \ddots & \ddots & -\alpha \\ 0 & & -\alpha & 2(\alpha+\beta) \end{pmatrix}.$$

- $-\beta\mathbf{I}$ represents coupling in the y-direction.
- Total size: $(N_x - 1)(N_y - 1) \times (N_x - 1)(N_y - 1)$.

c. Stencil Representation: The 5-point stencil for the generalized form:

$$\begin{bmatrix} & -\beta & \\ -\alpha & 2(\alpha+\beta) & -\alpha \\ & -\beta & \end{bmatrix}.$$

6. Verification of M-matrix:

- All off-diagonal entries of **A** are $-\alpha$ or $-\beta$, which are non-positive. Thus, $a_{ij} \leq 0$ for all $i \neq j$.
- **A** is strictly diagonally dominant:

$$|2(\alpha + \beta)| > | - \alpha| + | - \alpha| + | - \beta| + | - \beta| = 2\alpha + 2\beta.$$

- Diagonal dominance ensures **A** is non-singular.
- **A** is irreducibly diagonally dominant (due to the coupling between x and y directions).
- It is also positive definite (all eigenvalues are positive).
- For such matrices, the inverse is non-negative $(\mathbf{A}^{-1} \geq 0)$

Therefore **A** is M-matrix.

5.2 Inversion of Block Tridiagonal Matrices Using Chebyshev Polynomials

Block tridiagonal matrices frequently arise in the numerical solution of partial differential equations (PDEs) via finite difference methods. Efficient inversion of such matrices is crucial for computational efficiency. This work presents a symbolic method for inverting block tridiagonal matrices using Chebyshev polynomials of the second kind, which avoids direct numerical inversion and exploits recurrence relations for scalability.

Consider the second-order ODE with Dirichlet boundary conditions:

$$-\frac{d^2u}{dx^2} + qu = f(x), \quad q = Const, \quad u(0) = u(L) = 0$$

Discretizing on a uniform grid:

$$x_j = jh \quad (h = L/(n+1))$$

yields a linear system:

$$\mathbf{AU} = \mathbf{F}$$

The matrix **A** is a tridiagonal matrix of the form:

$$\mathbf{A}(z) = \begin{pmatrix} 2z & -1 & & & \\ -1 & 2z & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2z & -1 \\ & & & -1 & 2z \end{pmatrix} \in \mathbb{R}^{n\times n}, \quad z \in \mathbb{R}$$

where $z = 1 + h^2q/2$. Such matrices appear frequently in the finite difference discretization of second-order differential equations. Put $2z = a$, we get a tridiagonal matrix with diagonal entries a and off-diagonal entries -1.

$$\mathbf{A}(z) = \begin{pmatrix} a & -1 & & & \\ -1 & a & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & a & -1 \\ & & & -1 & a \end{pmatrix} \in \mathbb{R}^{n\times n}$$

The full matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ can be written in block form as:

$$\mathbf{A} = \begin{pmatrix} \mathbf{A}_0 & -\mathbf{I} & 0 & \cdots & 0 & 0 \\ -\mathbf{I} & \mathbf{A}_0 & -\mathbf{I} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \mathbf{A}_0 & -\mathbf{I} \\ 0 & 0 & 0 & \cdots & -\mathbf{I} & \mathbf{A}_0 \end{pmatrix}$$

where,

$$\mathbf{A}_0 = \begin{pmatrix} a & -1 & 0 \\ -1 & a & -1 \\ 0 & -1 & a \end{pmatrix}, \quad \mathbf{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The Chebyshev polynomials of the second kind $U_k(x)$ satisfy the recurrence relation:

$$U_0(x) = 1, \quad U_1(x) = 2x, \quad U_{k+1}(x) = 2x \cdot U_k(x) - U_{k-1}(x)$$

For $a = 2z$, we define:

$$\Delta_k = U_k\left(\frac{\mathbf{A}_0}{2}\right)$$

Explicitly, we have:

$$\begin{aligned} \Delta_0 &= \mathbf{I} \\ \Delta_1 &= \mathbf{A}_0 \\ \Delta_2 &= \mathbf{A}_0^2 - \mathbf{I} \\ \Delta_3 &= \mathbf{A}_0^3 - 2\mathbf{A}_0 \\ \Delta_4 &= \mathbf{A}_0^4 - 3\mathbf{A}_0^2 + \mathbf{I} \\ \Delta_5 &= \mathbf{A}_0^5 - 4\mathbf{A}_0^3 + 3\mathbf{A}_0 \end{aligned}$$

and so on ......

Then the inverse of **A** is given by:

$$\mathbf{A}^{-1} = \frac{\widetilde{\mathbf{D}}(z)}{\Delta_n(z)}, \quad \widetilde{\mathbf{D}}(z) = \begin{pmatrix} \Delta_{n-1}(z) & \Delta_{n-2}(z) & \cdots & \Delta_1(z) & \Delta_0(z) \\ \Delta_{n-2}(z) & & & & \Delta_1(z) \\ \vdots & \tilde{d}_{i,i-1} & \tilde{d}_{ii} & \tilde{d}_{i,i+1} & \vdots \\ \Delta_1(z) & & & & \Delta_{n-2}(z) \\ \Delta_0(z) & \Delta_1(z) & \cdots & \Delta_{n-2}(z) & \Delta_{n-1}(z) \end{pmatrix},$$

Alternatively, this can be written as:

$$\mathbf{A}^{-1} = [\Delta_n(z)]^{-1} \cdot \begin{pmatrix} \Delta_{n-1}(z) & \Delta_{n-2}(z) & \cdots & \Delta_1(z) & \Delta_0(z) \\ \Delta_{n-2}(z) & & & & \Delta_1(z) \\ \vdots & \tilde{d}_{i,i-1} & \tilde{d}_{ii} & \tilde{d}_{i,i+1} & \vdots \\ \Delta_1(z) & & & & \Delta_{n-2}(z) \\ \Delta_0(z) & \Delta_1(z) & \cdots & \Delta_{n-2}(z) & \Delta_{n-1}(z) \end{pmatrix}$$

where matrix $\tilde{D}(z) = (\tilde{d}_{ij})$ is symmetric and $\tilde{d}_{ij} = \tilde{d}_{i1}\tilde{d}_{nj} = \Delta_{n-i}\Delta_{j-1}$ for $j \leq i$.

5.3 Inversion of Block Tridiagonal Matrices using Kronecker product and eigenvalue Decomposition

$$-\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)=f(x,y)$$

Discretizing with step sizes hx and hy gives:

$$\frac{-u_{i-1,j}+2u_{i,j}-u_{i+1,j}}{h_x^2}+\frac{-u_{i,j-1}+2u_{i,j}-u_{i,j+1}}{h_y^2}=f_{i,j}$$

Combining terms

$$\frac{1}{h_x^2}(-u_{i-1,j}-u_{i+1,j})+\frac{1}{h_y^2}(-u_{i,j+1}-u_{i,j-1})+2\left(\frac{1}{h_x^2}+\frac{1}{h_y^2}\right)u_{i,j}=f_{i,j}$$

The linear system $\mathbf{AU}=\mathbf{F}$ has a block tridiagonal structure:

$$\mathcal{A}=\begin{bmatrix}\widetilde{\mathbf{A}} & -\widetilde{\mathbf{B}} & & & \\ -\widetilde{\mathbf{B}} & \widetilde{\mathbf{A}} & -\widetilde{\mathbf{B}} & & \\ & \ddots & \ddots & \ddots & \\ & & & & \widetilde{\mathbf{B}} \\ & & & \widetilde{\mathbf{B}} & \widetilde{\mathbf{A}}\end{bmatrix}$$

where

$$\widetilde{\mathbf{A}}=\begin{bmatrix}\widetilde{a} & -\widetilde{b} & & & \\ -\widetilde{b} & \widetilde{a} & -\widetilde{b} & & \\ & \ddots & \ddots & \ddots & \\ & & & & \widetilde{b} \\ & & & \widetilde{b} & \widetilde{a}\end{bmatrix}\quad \widetilde{a}=\frac{2}{h_x^2}+\frac{2}{h_y^2},\quad \widetilde{b}=\frac{1}{h_x^2}$$

$$\widetilde{\mathbf{B}}=\frac{1}{h_y^2}\mathbf{I}$$

$$\mathcal{A}=\frac{1}{h_y^2}\begin{bmatrix}\mathbf{A} & -\mathbf{I} & & & \\ -\mathbf{I} & \mathbf{A} & -\mathbf{I} & & \\ & \ddots & \ddots & \ddots & \\ & & & & -\mathbf{I} \\ & & & -\mathbf{I} & \mathbf{A}\end{bmatrix}\in\mathbb{Z}_n$$

$$\mathbf{A} = \frac{h_y^2}{h_x^2}\begin{bmatrix} a & -1 & & & \\ -1 & a & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & & & -1 \\ & & & -1 & a \end{bmatrix}, \quad a = 2(1+\frac{h_x^2}{h_y^2})$$

Step-by-step solution for the inverse using Kronecker product and eigenvalue Decomposition :

Step 1: Identify the matrix structure

$$\mathbf{A} = \mathbf{I}_N \otimes \mathbf{L}_M + \mathbf{L}_N \otimes \mathbf{I}_M$$

where $\mathbf{I}_N$ and $\mathbf{I}_M$ are identity matrices of sizes $N \times N$ and $M \times M$

$$\mathbf{L}_N = \frac{1}{h_x^2}\begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ 0 & -1 & 2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

$$\mathbf{L}_M = \frac{1}{h_y^2}\begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ 0 & -1 & 2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

Step2: Compute Eigenvalues of $\mathbf{L}_N$ and $\mathbf{L}_M$

The eigenvalues of $\mathbf{L}_N$ and $\mathbf{L}_M$ are known analytically:

$$\lambda_i(\mathbf{L}_N) = \frac{4}{h_x^2}\sin^2\left(\frac{i\pi h_x}{2}\right), \quad i = 1, \ldots, N-1$$

$$\lambda_j(\mathbf{L}_M) = \frac{4}{h_y^2}\sin^2\left(\frac{j\pi h_y}{2}\right), \quad j = 1, \ldots, M-1$$

step3: Eigenvalues of **A**

Using the property of Kronecker Sums:

$$\lambda(\mathbf{A}) = \lambda(\mathbf{I}_N \otimes \mathbf{L}_M + \mathbf{L}_N \otimes \mathbf{I}_M) \quad \forall i,j$$

$$= \lambda_i(\mathbf{L}_N) + \lambda_j(\mathbf{L}_M)$$

Thus the eigenvalue of **A** are

$$\lambda_{i,j}(\mathbf{A}) = \frac{4}{h_x^2}\sin^2\left(\frac{i\pi h_x}{2}\right) + \frac{4}{h_y^2}\sin^2\left(\frac{j\pi h_y}{2}\right)$$

Step 4: Eigenvectors of **A**

The eigenvectors of **A** are the Kronecker product of the eigenvectors of $\mathbf{L}_N$ and $\mathbf{L}_M$:

$$\mathbf{V}_A = \mathbf{V}_N \otimes \mathbf{V}_M$$

where $\mathbf{V}_N$ and $\mathbf{V}_M$ are matrices of eigenvectors of $\mathbf{L}_N$ and $\mathbf{L}_M$.

Step 5: Construct $\mathbf{A}^{-1}$ via diagonalization.

$$\mathbf{A}^{-1} = (\mathbf{V}_N \otimes \mathbf{V}_M) \cdot \left[\text{diag}(\Lambda_{ij}^{-1})\right] \cdot (\mathbf{V}_N^T \otimes \mathbf{V}_M^T)$$

where

$$\Lambda_{ij}^{-1} = \left[\frac{4}{h_x^2}\sin^2\left(\frac{i\pi h_x}{2}\right) + \frac{4}{h_y^2}\sin^2\left(\frac{j\pi h_y}{2}\right)\right]^{-1}$$

Verification of M-Matrix Properties:

A matrix is a Z-matrix if all its off-diagonal entries are non-positive.

- The diagonal entries of **A** are $\frac{2}{h_x^2} + \frac{2}{h_y^2} > 0$.
- The off-diagonal entries are $-\frac{1}{h_x^2}$ and $-\frac{1}{h_y^2} < 0$.

So, **A** is a Z-matrix.

An M-matrix must be invertible with $\mathbf{A}^{-1} \geq 0$.

The eigenvalues of **A** are:

$$\lambda_{i,j}(\mathbf{A}) = \frac{4}{h_x^2}\sin^2\left(\frac{i\pi h_x}{2}\right) + \frac{4}{h_y^2}\sin^2\left(\frac{j\pi h_y}{2}\right) > 0 \quad \forall i,j.$$

Since all eigenvalues are positive, **A** is invertible.

The inverse is constructed via:

$$\mathbf{A}^{-1} = (\mathbf{V}_N \otimes \mathbf{V}_M) \cdot \text{diag}(\Lambda_{ij}^{-1}) \cdot (\mathbf{V}_N^T \otimes \mathbf{V}_M^T),$$

where:

- The eigenvectors (discrete sine functions) are non-negative.
- The eigenvalues Λ_{ij}^{-1} are positive.

So, $\mathbf{A}^{-1} \geq 0$.

Finally, **A** is an M-matrix.

5.4 Applications

The discovery of the spectral radius of the matrix R, which is used to demonstrate that the matrix A is an M-matrix, is one of the most important new findings presented in the thesis. In addition to providing both necessary and sufficient criteria, the method is founded on the principle of regular splitting.

To prove this applications of M-matrix, we solve the two-dimensional Poisson equation numerically. To do this, we first discretize the equation using finite differences on a grid with step sizes h_x (x-direction) and h_y (y-direction). For a typical interior grid point $(U_{1,1})$, we consider its neighbors: U_b (a boundary point), $U_{2,1}$ (right neighbor), U_{up} (upper neighbor), and U_{down} (lower neighbor). Applying the boundary condition $U_b = \gamma u(i)$ and assuming $U_{down} = 0$, the discretized equation simplifies to

$$-\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = f(x,y),$$

$$-\left(\frac{U_b - 2U_{11} + U_{21}}{h_x^2}\right) - \left(\frac{U_{up} - 2U_{11} + U_{down}}{h_y^2}\right) = f_{ij}$$

$$-\left(\frac{\gamma u_i - 2U_{11} + U_{21}}{h_x^2}\right) - \left(\frac{U_{up} - 2U_{11}}{h_y^2}\right) = f_{ij}$$

$$-\frac{\gamma u_i}{h_x^2} + \frac{2U_{11}}{h_x^2} - \frac{U_{21}}{h_x^2} - \frac{U_{up}}{h_y^2} + \frac{2U_{11}}{h_y^2} = f_{ij}$$

Diagonal entry:

$$\frac{2}{h_x^2} + \frac{2}{h_y^2} - \frac{\gamma}{h_x^2}$$

off diagonal:

$$-\frac{1}{h_x^2} \text{ for } U_{21} \quad (x - neighborhood)$$

$$-\frac{1}{h_y^2} \text{ for } U_{up} \quad (y - neighbor)$$

This forms a linear system where the resulting system matrix is an M-matrix. This special property guarantees that iterative numerical methods will converge to a stable solution.

The linear system **AU** $=$ **F** is constructed as follows:

$$A_i = \frac{1}{h^2}\begin{bmatrix} 4-\gamma & -1 & & \\ -1 & 4 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 4 \end{bmatrix}_{n\times n}$$

Here we take example of 12×12:

$$A_i = \frac{1}{h^2} \begin{bmatrix} 4-\gamma & -1 & & \\ -1 & 4 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 4 \end{bmatrix}_{12\times 12} , \quad C = \frac{1}{h^2} \begin{bmatrix} \gamma & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}_{12\times 12}$$

Determine for which values of γ the matrix $A = A_i - C$ remains an M-matrix.
Step 1: Verify A_i is an M-matrix when $\gamma = 0$,

$$A_i = \frac{1}{h^2} \begin{bmatrix} 4 & -1 & & \\ -1 & 4 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 4 \end{bmatrix}_{12\times 12}$$

$$A_i^{-1} = \frac{1}{h^2} \begin{pmatrix} 0.29 & 0.09 & 0.03 & 0.10 & 0.06 & 0.02 & 0.03 & 0.03 & 0.01 & 0.01 & 0.01 & 0.01 \\ 0.09 & 0.33 & 0.09 & 0.06 & 0.12 & 0.06 & 0.03 & 0.05 & 0.03 & 0.01 & 0.02 & 0.01 \\ 0.03 & 0.09 & 0.29 & 0.02 & 0.06 & 0.10 & 0.01 & 0.03 & 0.03 & 0.01 & 0.01 & 0.01 \\ 0.10 & 0.06 & 0.02 & 0.33 & 0.13 & 0.04 & 0.11 & 0.07 & 0.03 & 0.03 & 0.03 & 0.01 \\ 0.06 & 0.12 & 0.06 & 0.13 & 0.38 & 0.13 & 0.07 & 0.14 & 0.07 & 0.03 & 0.05 & 0.03 \\ 0.02 & 0.06 & 0.10 & 0.04 & 0.13 & 0.33 & 0.03 & 0.07 & 0.11 & 0.01 & 0.03 & 0.03 \\ 0.03 & 0.03 & 0.01 & 0.11 & 0.07 & 0.03 & 0.33 & 0.13 & 0.04 & 0.10 & 0.06 & 0.02 \\ 0.03 & 0.05 & 0.03 & 0.07 & 0.14 & 0.07 & 0.13 & 0.38 & 0.13 & 0.06 & 0.12 & 0.06 \\ 0.01 & 0.03 & 0.03 & 0.03 & 0.07 & 0.11 & 0.04 & 0.13 & 0.33 & 0.02 & 0.06 & 0.10 \\ 0.01 & 0.01 & 0.01 & 0.03 & 0.03 & 0.01 & 0.10 & 0.06 & 0.02 & 0.29 & 0.09 & 0.03 \\ 0.01 & 0.02 & 0.01 & 0.03 & 0.05 & 0.03 & 0.06 & 0.12 & 0.06 & 0.09 & 0.33 & 0.09 \\ 0.01 & 0.01 & 0.01 & 0.01 & 0.03 & 0.03 & 0.02 & 0.06 & 0.10 & 0.03 & 0.09 & 0.29 \end{pmatrix}$$

Properties:

- Z-matrix: All off-diagonal entries are non-positive ($-1 \leq 0$)
- Diagonally dominant:
  - For interior rows: $4 \geq |-1| + |-1| = 2$
  - For boundary rows: $4 \geq |-1| = 1$
- Inverse non-negative: Numerically computed $A_i^{-1} \geq 0$.

Step 2. Regular Splitting: The splitting $A = A_i - C$ is a regular splitting because:

- A_i is an M-matrix ($\gamma = 0$ case)
- $C \geq 0$ (since $\gamma \geq 0$ and $h^2 > 0$)

Step 3: Compute $R = (A_i)^{-1}C$ and $\rho(R)$ Given the structure of C, R has only the first column non-zero:

$$R = (A_i)^{-1}C = \frac{\gamma}{h^2}\begin{bmatrix} (A_i^{-1})_{11} & 0 & \cdots & 0 \\ (A_i^{-1})_{21} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ (A_i^{-1})_{12,1} & 0 & \cdots & 0 \end{bmatrix}$$

The spectral radius $\rho(R)$ is:

$$\rho(R) = \frac{\gamma}{h^2}(A_i^{-1})_{11}$$

From the provided A_i^{-1}:

$$(A_i^{-1})_{11} = 0.29h^2$$

Thus:

$$\rho(R) = \gamma \cdot 0.29$$

Step 4: For A to be an M-matrix, we require:

$$\rho(R) < 1 \implies \gamma \cdot 0.29 < 1 \implies \gamma < \frac{1}{0.29} \approx 3.448$$

The matrix $A = A_i - C$ remains an M-matrix if and only if:

$$\boxed{\gamma < \frac{1}{0.29} \approx 3.448}$$

Results and conclusions

We established a theoretical framework linking M-matrix spectral properties to Chebyshev polynomial solvers. Our resulting algorithms combine these concepts, achieving faster convergence than standard methods. For large sparse systems from elliptic PDEs, the proposed solvers and preconditioners cut computing costs (fewer iterations, less time) and remained stable in practice. Integrating matrix algebra with polynomial approximation significantly enhances numerical method robustness and efficiency. Future work could extend this to more complex PDE systems and test adaptive techniques. The research employed a range of mathematical, numerical, and application-oriented datasets to analyze how M-matrices and Chebyshev polynomials influence finite difference methods. Sparse, structured matrices were utilized to confirm the M-matrix characteristics essential for stability, while coefficients derived from Chebyshev polynomials contributed to higher numerical precision. Grid configurations and step size adjustments were instrumental in achieving stable discretized models. The methodology was rigorously tested against established benchmark solutions to verify its effectiveness. Quantitative error measurements indicated enhanced convergence rates, and computational efficiency metrics demonstrated the method's practical advantages. Collectively, the findings highlight that integrating M-matrix principles with Chebyshev polynomial techniques substantially improves the robustness, precision, and dependability of finite difference approaches for solving differential equations.

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