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Stochastic Numerical Methods for Eigenvalue Estimation

A B S T R A C T

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The dissertation contains **118** pages and includes **15** figures and **16** tables, as well as a list of the mathematical notation and abbreviations used. The dissertation consists of an introduction, three main chapters, a conclusion, a list of publications, an approbation of the results, formulation of the scientific and applied contributions, an appendix, and **10** pages of a bibliography comprising **121** references.
The public defense of the dissertation will take place on **.....** at **.....** in hall **218** of block 25A of IICT-BAS at an open meeting of the scientific jury composed of:

Scientific jury:

1. .....
2. .....
3. .....
4. .....
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6. .....

The reviews and opinions of the members of the scientific jury and the abstract are published on the IICT-BAS website.
The materials for the defense are available for those interested at the following address: IICT-BAS, Acad. G. Bonchev Str., block 2, floor 3, room ....

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Title: **Stochastic Numerical Methods for Eigenvalue Estimation**

General Characteristic of the Dissertation

Relevance of the Topic

The problem of finding and estimating extreme eigenvalues of square, in particular symmetric, matrices occupies a central place in linear algebra due to its key role in a wide range of scientific and applied fields. Such problems arise in quantum mechanics, where, in the Schrödinger equation [65], the eigenvalues of the Hamiltonian operator determine the energy spectrum of the system, and the extreme values provide information about the ground and excited states [64, 73]. In financial mathematics, the analysis of extreme eigenvalues of covariance matrices is essential for risk modeling and portfolio optimization, including the assessment of systematic market risk and diversification opportunities [51, 72]. In spectral graph theory, these values are associated with structural properties such as connectivity, expansion, and robustness, which are decisive for the efficiency of algorithms in machine learning and network analysis [8, 12, 26]. In image processing and computer vision, eigenvalues play a crucial role in principal component analysis, dimensionality reduction, noise suppression, and spectral segmentation [47, 34]. In tensor analysis and multidimensional data processing, the maximum eigenvalue and spectral norms determine the behavior of iterative methods and regularization techniques, with applications in signal processing and artificial intelligence [49, 56, 80].

There exist various numerical approaches for computing eigenvalues and eigenvectors: exact (direct), iterative, and stochastic. Direct methods include the QR decomposition and solving the characteristic polynomial for small dimensions. They provide a solution in a finite number of steps and have computational complexity of order $\mathcal{O}(n^3)$. In high dimensions, they suffer from the accumulation of numerical errors due to rounding in arithmetic operations [87, 90].

Iterative methods, such as the power method, inverse power method, Jacobi method, and the Arnoldi and Lanczos methods [33, 43], have lower computational complexity $\mathcal{O}(n^2k)$, where n is the matrix dimension and k is the number of iterations. However, these methods are often characterized by slow convergence, strong dependence on the initial approximation, significant memory requirements, and limited parallel efficiency.

Stochastic numerical methods offer an effective alternative by providing linear dependence of the required memory on the problem dimension, as well as natural parallelism and relative ease of implementation. Although they exhibit slower convergence and lower precision than deterministic methods, they enable the solution of very high-dimensional problems. They are particularly well-suited for estimating extreme eigenvalues of symmetric matrices.

In the context of the rapid development of high-performance computing (HPC) systems and the emergence of new hardware architectures, there is a growing need for the development and deployment of software solutions based on efficient stochastic algorithms for high-dimensional problems, including the estimation of extreme eigenvalues [18, 24, 59]. This has led to increased research interest in improving accuracy, accelerating convergence, and expanding the applicability of stochastic methods in scientific computing, machine learning, and data analysis, aligned with modern computational capabilities.

Overview of the Main Results in the Field

The earliest publications on Monte Carlo (MC) methods in linear algebra date back to the 1950s and 1960s, and they did not initially address the problem of approximate eigenvalue computation. The task of finding the eigenvalues and eigenvectors of matrices usually arises when solving systems of linear algebraic equations (LAEs) and stochastic differential equations (SDEs). In practice, for high-dimensional matrices, it is usually necessary to compute only the extreme eigenvalues, which determine the condition number and key properties of the system [63, 87, 90]. Such problems arise in image and signal processing, control systems, machine learning, and quantum mechanics, where, for example, the energy levels of quantum systems are determined by the eigenvalues of the Hamiltonian operator [64, 73]. In addition to these, deterministic methods such as the power method, the Rayleigh quotient iteration, the resolvent power method, and the Lanczos algorithm are widely used [33, 43].

The Monte Carlo method for estimating the dominant eigenvalue was proposed by Sobol in 1973 [92], while Mikhailov introduced the method for the smallest eigenvalue in 1987 [55]. Significant contributions to the development of the Power Monte Carlo (PMC) method were made by Dimov and Karaivanova during the period 1996-2000 [15, 18, 21, 23, 24, 25]. In the following decades, iterative MC and Quasi-Monte Carlo (QMC) algorithms were developed to find extreme eigenvalues, based on the power and resolvent power methods [3, 19, 21, 25, 60]. In particular, the use of the resolvent matrix to estimate the smallest eigenvalue was introduced by Dimov and Karaivanova in 1998 [24].

The first QMC method for finding extreme eigenvalues were proposed by Karaivanova and Mascagni in the period 2001–2003 [58, 59, 60, 61]. A number of studies have used QMC methods based on low-discrepancy sequences, including the Sobol sequences [74, 75, 76], the Halton sequences [39, 40], and the Faure sequences [28, 29, 30], providing a more uniform and deterministic coverage of the sample space [2, 3, 10, 11, 44, 48]. Compared to MC approaches, QMC methods are distinguished by greater flexibility, applicability to large-scale matrices, relative simplicity, and efficient parallelization [16, 22, 61].
Over the past two decades, various strategies for parallelizing MC algorithms have been developed and analyzed [4, 5, 6, 78, 79, 83]. Parallel MC methods for solving systems of linear algebraic equations based on the Jacobi iteration have been presented by Dimov [16], as well as approaches using minimal Markov chains and minimal communication [27, 82]. A key idea in these developments is the balancing of stochastic and systematic errors [16]. Hybrid MC algorithms for matrix computations have also been developed [1, 84], including parallel implementations to estimate the largest and smallest eigenvalues of matrices proposed by Dimov, Mascagni and Karaivanova [20, 24, 59].

Goals and Tasks of the Dissertation

The main goal of the dissertation is to propose and investigate stochastic numerical methods for estimating eigenvalues and to develop and analyze Monte Carlo and randomized Quasi-Monte Carlo algorithms to approximate the extreme eigenvalues of symmetric square matrices. To achieve the main goal, the following tasks have been formulated.

1. Consider and study the Power (Resolvent) Monte Carlo method and the randomized Power (Resolvent) QMC method for estimating the extreme eigenvalues of symmetric matrices, and analyze the balance between the resulting stochastic and systematic errors.

2. Develop and investigate efficient Monte Carlo and randomized Quasi-Monte Carlo algorithms based on these stochastic methods for numerically calculating the extreme eigenvalues of symmetric square matrices, using generators of pseudorandom numbers and low-discrepancy sequences.

3. Conduct numerical experiments with the developed algorithms, justifying the choice of specialized software for generating low-discrepancy sequences, in particular, Sobol and Halton sequences, and to numerically investigate the balance between stochastic and systematic error depending on their defining parameters.

4. Formulate and investigate a problem in the field of financial mathematics related to the management of the market risk of an asset portfolio, in which the risk assessment is based on the determination of the maximum eigenvalue of a correlation matrix. Apply the Power Monte Carlo (PMC) and randomized Power Quasi-Monte Carlo (PQMC) algorithms developed in Chapter 1 to numerically estimate the largest eigenvalue and to analyze their effectiveness in assessing market risk.

Research Methodology

The research methodology in this dissertation is based on fundamental scientific results in the following areas:

- Probability theory and mathematical statistics - probability spaces; random variables and their characteristics such as distribution functions, probability density function, mathematical expectation, variance; law of large numbers; central limit theorem; probability error, confidence interval, Markov chain; samples of random variables; statistical tests for studying generators of pseudorandom variables.

- Mathematical analysis - series and sequences, convergence of series, convergence criteria, systematic error, norms, and metric spaces.

- Numerical methods, linear and computational algebra - iterative methods for SLAE and eigenvalues; matrix norms; optimization methods; algorithms for generating pseudorandom numbers, stochastic numerical methods (Monte Carlo and Quasi-Monte Carlo methods).

- Number theory, more precisely, discrete and analytic number theory - uniformly distributed sequences, discrepancy, radical-inverse functions, decomposition into prime bases.

- Computer science - algorithms and data structures; programs/codes written in MATLAB, C++ using pseudo-random number generators such as MT and MS; libraries for randomized Sobol and Halton sequences.

Part of the numerical experiments were performed on the high-performance cluster, which consists of 12 Fujitsu Primergy RX 2540 M4 servers. Each server is configured with an NVIDIA Tesla V100 32GB GPU and two x Intel Xeon Gold 5118 2.30 GHz, 24 CPU cores, with 128 GB RAM. The Sobol sequences were obtained using BRODA's Sobol Randomized Sequence Generator (RSG) [7].
In the following sections, we have formulated the basic problem of estimating eigenvalues of a symmetric matrix and described the MC and QMC approaches for numerically solving multidimensional problems, along with the errors that characterize these methods.

Problem Formulation

Consider a matrix $A = \{a_{ij}\}_{i,j=1}^{n} \in \mathbb{R}^{n\times n}$, with $a_{ij} = a_{ji}$, $i, j = 1, \ldots, n$. The problem of finding the eigenvalues $\lambda(A)$ is formulated as follows:

$$A\boldsymbol{x} = \lambda\boldsymbol{x}, \text{ where } \boldsymbol{x} \in \mathbb{R}^n \text{ is an arbitrary nonzero vector.} \tag{1}$$

All eigenvalues of symmetric matrices are real numbers. Without loss of generality, the following ordering is assumed:

$$\lambda_{min} = |\lambda_n| \leq |\lambda_{n-1}| \leq \ldots \leq |\lambda_2| < |\lambda_1| = \lambda_{max}. \tag{2}$$

The matrix A can also be represented in vector form as:

$$A = \{a_{ij}\}_{i,j=1}^{n} = (\boldsymbol{a}_1, \ldots, \boldsymbol{a}_i, \ldots, \boldsymbol{a}_n)^T, \text{ where } \boldsymbol{a}_i = (a_{i1}, \ldots, a_{in}),\ i = 1, \ldots, n.$$

The symbol T denotes the transpose operation. For this study, the following vector and matrix norms are used:

$$\|\boldsymbol{h}\| = \|\boldsymbol{h}\|_1 = \sum_{i=1}^{n} |h_i|,\ \ \|\boldsymbol{a}_i\| = \|\boldsymbol{a}_i\|_1 = \sum_{j=1}^{n} |a_{ij}|,\ \ \|A\| = \|A\|_1 = \max_j \sum_{i=1}^{n} |a_{ij}|,\ \ j = 1, \ldots, n.$$

The application of stochastic numerical methods to estimate the extreme eigenvalues λ_{min} and λ_{max} of the problem defined above involves developing and analysing Power (Resolvent) Monte Carlo and randomized Power (Resolvent) Quasi-Monte Carlo algorithms for their approximate computation. By stochastic numerical methods, we will further understand Monte Carlo methods and their variants, the randomized Quasi-Monte Carlo methods.

Monte Carlo Methods

Monte Carlo (MC) methods are based on the construction of a random variable (r.v.) θ, which is in fact a measurable function $\theta = \theta(\omega)$ defined on the probability space $(\Omega, \mathfrak{A}, \mathbb{P})$ [88], with domain Ω and range $\mathbb{R}$ (the set of real numbers). The condition in constructing the random variable θ is related to its mathematical expectation. The requirement is that the mathematical expectation should equal the desired solution to a given problem or a functional of the solution to the original problem.

$$E[\theta] = I, \tag{3}$$

where I is the sought solution. By definition, $E[\theta]$ exists if and only if $E|\theta|$ exists.
Depending on the specific problem, the random variable θ may be discrete or continuous. In the discrete case, the expectation is given by:

$$E[\theta(\omega)] = \sum_i \mathbb{P}\{\theta(\omega) = x_i)\}x_i = \sum_i p_i x_i = I, \text{ where } \sum_i p_i = 1,$$

and in the continuous case:

$$E[\theta] = \int_{-\infty}^{\infty} xp(x)\ dx, \text{ where } \int_{-\infty}^{\infty} p(x)\ dx = 1,$$

where $p(x) \geq 0$ is the probability density function. The distribution function $F_\theta(x) = \mathbb{P}\{\theta < x\}$ describes the cumulative probability and is related to $p(x)$ through standard differential relationships [88, 91].
When implementing an MC algorithm, a sample $\theta_1, \theta_2, \ldots, \theta_N, \ldots$ is generated from identically distributed independent realizations of the random variable θ, and the approximate value of I is determined by the mean:

$$\overline{\theta}_N = \frac{1}{N}\sum_{i=1}^{N}\theta_i. \tag{4}$$

Convergence and Error Estimation in Monte Carlo Methods

The theoretical justification of MC methods is based on the Law of Large Numbers (LLN). When the mathematical expectation is finite, the sequence of mean values $\overline{\theta}_N$ converges in probability to I as $N \to \infty$ (The Weak Law of Large Numbers, Khinchin's theorem) [14, 88]. The necessary and sufficient condition for the convergence to be almost sure (Strong Law of Large Numbers, Kolmogorov's theorem) is that there is a mathematical expectation.
Suppose that the random variable θ has finite variance, i.e.

$$Var[\theta] = E[\theta - E\theta]^2 = E[\theta^2] - (E[\theta])^2 < \infty.$$

Then the Central Limit Theorem (CLT) ensures an asymptotically normal distribution of the error [31, 88]. As a result, the following probabilistic estimate is obtained:

$$\lim_{N\to\infty} \mathbb{P}\left\{\left|\frac{1}{N}\sum_{i=1}^{N}(\theta_i - I)\right| < x\sigma N^{-1/2}\right\} = \Phi(x),$$

where $\sigma = \sqrt{Var[\theta]}$, and $\Phi(x) = \dfrac{2}{\sqrt{2\pi}}\displaystyle\int_0^x e^{-\frac{t^2}{2}}dt$ is called the probability integral and is determined by the distribution function of a standard normal random variable in the interval $(0, 1)$ [92].
The quantity

$$r_N = x_\beta \sigma N^{-\frac{1}{2}} \tag{5}$$

is called the probability error, with the parameter β determining the level of confidence. At $\beta = 0.5$, the so-called probability error is obtained, which characterizes the typical convergence rate of MC methods of the order of $\mathcal{O}(N^{-1/2})$.
In practical applications, the variance of the random variable θ is empirically estimated by the formula:

$$Var[\theta] \approx \frac{1}{N}\sum_{i=1}^{N}(\theta_i)^2 - (\overline{\theta}_N)^2. \tag{6}$$

When the sample size N of random variable values is small, the more accurate formula is usually used [92]:

$$Var[\theta] \approx \frac{1}{(N-1)}\sum_{i=1}^{N}(\theta_i)^2 - \frac{N}{N-1}(\overline{\theta}_N)^2. \tag{7}$$

Two types of MC methods are distinguished to reduce error [22, 89, 92]:

- Efficient MC methods, which aim to minimize the variance through variance reduction techniques (separation of a principal part, symmetrization of the subintegral function, essential sample method, importance partitioning method, etc.), without changing the asymptotic order of the error.
- Superconvergent MC methods, in which by sampling the values of a random variable in uniform non-overlapping subdomains and under additional conditions for smoothness of the subintegral function, a higher order of convergence is achieved $r_N = \mathcal{O}(N^{-1/2-\varepsilon(k)})$, where $\varepsilon(k) > 0$ depends on the dimensionality of the problem.

Pseudorandom number generators are used to simulate the values of random variables.

Pseudorandom Number Generators

The practical implementation of MC methods requires the use of pseudorandom number generators (PRNGs), which generate uniformly distributed values in $(0, 1)$ [53, 81]. The main requirements for good PRNGs include statistical randomness, a long period, reproducibility, efficiency, and the ability to generate in parallel [50, 53]. Among the most commonly used generators are linear and combined congruential generators [32, 54, 71], shift register generators (e.g., Mersenne Twister [62]), and generators based on other mathematical constructs

(e.g., Middle Square PRNG [70]). In the dissertation research for the implementation of stochastic algorithms for estimating extreme eigenvalues, Mersenne Twister (MT) and Middle Square (MS) pseudorandom number generators were used.

Quasi-Monte Carlo Methods

Quasi–Monte Carlo (QMC) methods are a deterministic alternative to Monte Carlo (MC) methods and use low-discrepancy sequences instead of pseudorandom points [39, 66, 74]. They provide a more uniform coverage of the unit hypercube $[0,1]^k$ and lead to improved convergence rates of order $\mathcal{O}(N^{-1}(\log N)^k)$, provided the integrand is sufficiently smooth [9, 52]. When estimating multidimensional integrals, the approximate solution has the form:

$$\int_{[0,1]^k} f(x)dx \approx \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i), \tag{8}$$

where $\mathbf{x}_i$ are elements of a low-discrepancy sequence.

Low-Discrepancy Sequences and Error Estimation

The key characteristic of these sequences is the star-discrepancy $D_N^*(S)$, which measures the deviation from a uniform distribution:

$$D_N^*(S) = \sup_{\mathbf{z}\in[0,1)^k} \left| \frac{1}{N}\sum_{i=1}^{N} \mathbf{1}_Z(\mathbf{x}_i) - \prod_{j=1}^{k} z_j \right|. \tag{9}$$

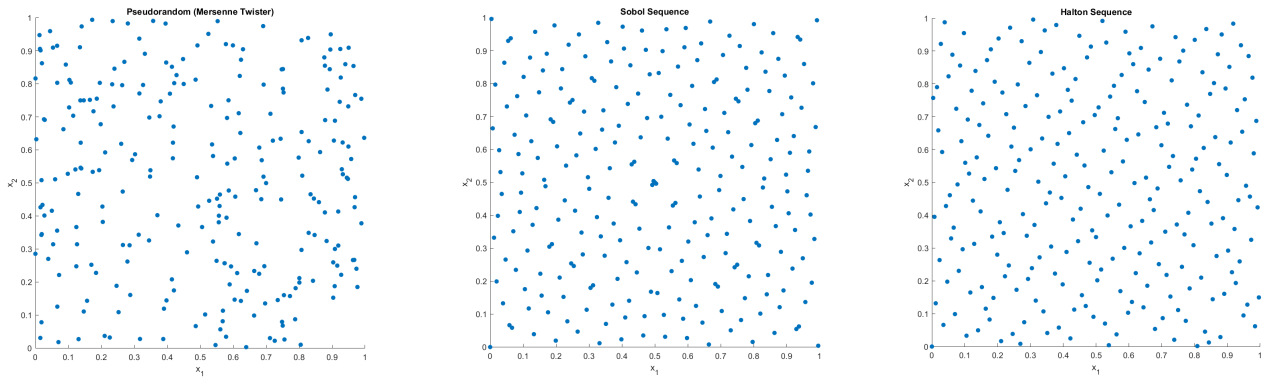
A sequence is said to have low-discrepancy if

$$D_N(S) = \mathcal{O}(N^{-1}(\log N)^k) \text{ or } D_N(S) \leq C_k \frac{(\log N)^k}{N}, \tag{10}$$

where the constant C_k in (10) depends only on the dimension k.
The error in Quasi-Monte Carlo (QMC) methods is estimated using the Koksma–Hlawka inequality [9, 72]:

$$\left| I(f) - \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i) \right| \leq V(f) D_N^*(S), \tag{11}$$

where $D_N^*(S)$ is the star-discrepancy of the sequence $S = \{\mathbf{x}_i\}_{i=1}^{\infty} \in [0,1)^k$. $V(f)$ is the variation of the function in the sense of Hardy-Krause. This inequality shows that the error depends on both the smoothness of the integrand and on the uniformity of the point sequence used. For sufficiently smooth functions, an asymptotic error order of $\mathcal{O}(N^{-1}(\log N)^k)$ is achieved, which is theoretically better than that of classical MC methods.



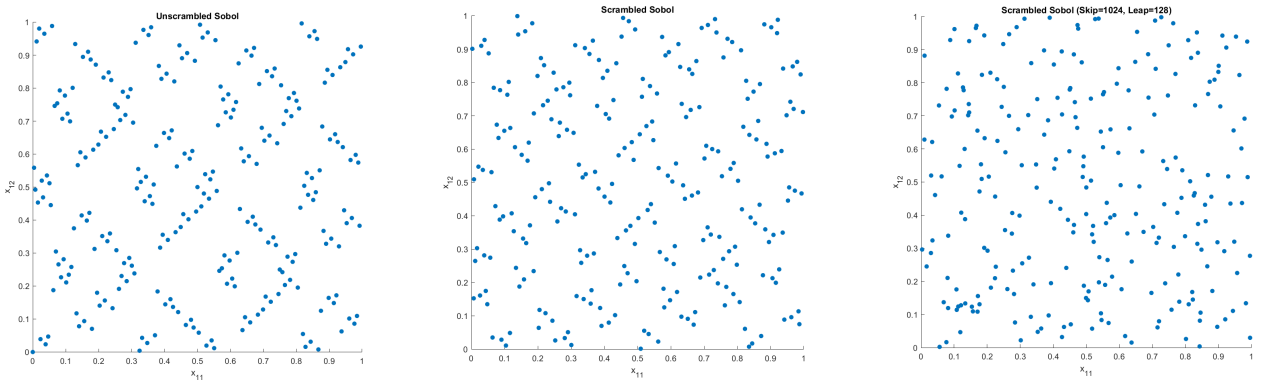
(a) MT pseudorandom number generator (b) Sobol sequence (c) Halton sequence

Figure 1: Comparison of a two-dimensional pseudorandom sequence generated with an MT PRNG with two-dimensional projections of the 16-dimensional Sobol and Halton sequences. 256 points are generated, and the projection is made along the first two coordinates.

The first constructions of low-discrepancy sequences originate from the van der Corput sequence [85]. Halton extended this idea to the multidimensional case by using radical inversion in different prime bases for each coordinate [39]. Halton sequences are conceptually simple, but in higher dimensions they may exhibit correlations, which necessitates the use of modifications [41, 86]. Sobol sequences, introduced in 1976 [76], are digital (t, k)-sequences in base 2. They are constructed using direction numbers derived from primitive polynomials over the finite field $\mathbb{F}_2 = \{0, 1\}$ (with addition modulo 2), which ensures high uniformity and good projection properties [74, 89]. Due to these properties, Sobol sequences are among the most widely used in QMC applications.
Figure (1) presents a comparison between a two-dimensional pseudorandom sequence generated by the Mersenne Twister (MT) and two-dimensional projections of 16-dimensional Sobol and Halton sequences. A clearly more uniform coverage of the unit square is observed for the low-discrepancy sequences compared to the pseudorandom sequence.

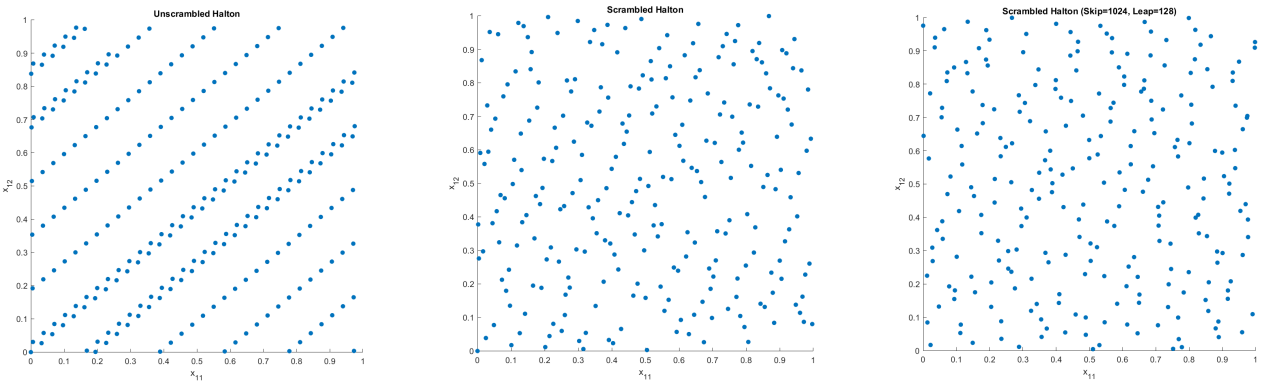
Scrambled Low-Discrepancy Sequences

The deterministic nature of classical low-discrepancy sequences leads to the absence of a natural probabilistic framework for error estimation and to the risk of correlations in high dimensions. These drawbacks are addressed by introducing scrambled (randomized) low-discrepancy sequences, in which controlled stochasticity preserves the uniform coverage of the unit hypercube while overcoming the limitations of fixed geometry [13].



(a) non-scrambled Sobol sequence (b) scrambled Sobol sequence (c) scrambled Sobol sequence with parameters *skip, leap*

Figure 2: Comparison between a two-dimensional projection with the presence of correlation in the 11th and 12th coordinates of the Sobol sequence and the corresponding two-dimensional projections of the scrambled Sobol sequence without and with the additionally included the parameters $skip = 1024$ and $leap = 128$.



(a) non-scrambled Halton sequence (b) scrambled Halton sequence (c) scrambled Halton sequence with the parameters *skip, leap*

Figure 3: Comparison between a two-dimensional projection with the presence of correlation at the 11th and 12th coordinates of the Halton sequence and the corresponding two-dimensional projections of the scrambled Halton sequence without and with the additional the parameters $skip = 1024$ and $leap = 128$.

In addition to scrambled low-discrepancy sequences, techniques can be used to skip initial elements of the sequence by applying a skipping operator and a leaping operator. In this way, the low-discrepancy property is preserved, while introducing controlled randomness, allowing statistical error estimation.
Figures (2) and (3) demonstrate the presence of correlations in non-scrambled Sobol and Halton sequences in higher coordinates, as well as the effect of applying the scrambling method. Scrambling leads to a significant improvement in the uniformity of the point distribution, as shown in Figure (2b) and Figure (3b). Figure (2c) and Figure (3c) also illustrate the additional effect of combining scrambling with the *skip* and *leap* parameters. These techniques reduce correlations and improve the practical performance of sequences in higher-dimensional problems.
Modern modifications of the Halton and Sobol sequences include randomization aimed at reducing correlations and improving convergence [52, 66] for specific problems. Randomization is implemented by applying specially constructed transformations (scramblings) to already established low-discrepancy sequences. There are two main approaches to scrambling. The first is based on random permutations of digits, where the digits of the coordinates in the base b (in particular, the base 2 in binary representation) are subjected to random permutations [67]. The second approach is based on addition modulo 1 with a random number or a random vector generated by a pseudorandom generator. This method is also known as random shifting (or shift) modulo 1 and is characterized by a simple and efficient implementation [45, 46]. In practice, the two approaches are often combined, leading to numerous variants and hybrid techniques [69, 68].

Stochastic Methods with Markov Chains

Monte Carlo (MC) and Quasi-Monte Carlo (QMC) methods are conventionally classified into two main groups: direct and iterative.
Direct MC/QMC methods are characterized by the fact that the approximate solution is influenced solely by stochastic (statistical) error. In the classical MC approach, this error is of order $\mathcal{O}(N^{-1/2})$ and is estimated via the inequality (5). In contrast, in QMC methods it is described by the Koksma–Hlawka inequality (11) and has asymptotic order $\mathcal{O}\big(N^{-1}(\log N)^k\big)$ when low-discrepancy sequences such as Sobol and Halton sequences are used. In this dissertation, randomized low-discrepancy sequences are employed to achieve more uniform coverage of the unit cube while maintaining controlled stochasticity. Therefore, the errors estimated by (5) and (11) are interpreted as stochastic errors depending on the sample size N.
Iterative MC/QMC methods, in addition to stochastic error, also include a systematic error, since they do not estimate the exact solution directly but rather a finite iteration of a convergent iterative process. As with classical numerical methods in linear algebra, such as the simple iteration method and the Gauss–Seidel method [90], the systematic error depends on the properties of the iterative scheme and the norm of the matrix involved. In stochastic iterative methods for linear algebra problems, a random variable $\theta^{(k)}$ is constructed by a Markov chain with k transitions [16, 22, 92]. The number of transitions can be fixed or random, with a mathematical expectation of k. The mathematical expectation of the random variable $\theta^{(k)}$ approximates the desired solution by a functional involving matrix-vector products. In this context, the systematic error is determined by the number of iterations k, while the stochastic error depends on the sample size N. Therefore, balancing systematic and stochastic errors and reducing variance are fundamental research tasks in the development of efficient stochastic iterative methods and algorithms for linear algebra.

Structure of the Dissertation

The dissertation is structured into an introduction, three chapters, a conclusion, an appendix, and a bibliography. It contains 118 pages, including 15 figures and 16 tables, a bibliography of 121 references, and a list of mathematical notation and abbreviations.

- The **Introduction** presents the relevance of the topic, provides an overview of the main scientific results in the field, defines the aims and objectives of the dissertation, and describes in detail the research methodology.
- **Chapter 1** Stochastic Power Method: Development and Analysis of Efficient Algorithms for Estimating the Maximum Eigenvalue is devoted to developing efficient stochastic power algorithms for estimating the maximum eigenvalue of dense symmetric matrices. The problem is defined, and the methods used to solve it are considered: the stochastic Power Method in two variants, Power Monte Carlo (PMC) and Power Quasi-Monte Carlo (PQMC). The construction of a random variable using a Markov chain is described in detail, with emphasis on the use of almost optimal probabilities. The pseudocode of the almost optimal PMC and PQMC algorithms developed is presented and conditions are determined to balance stochastic

and systematic errors. The chapter concludes with a discussion of numerical experiments conducted on matrices of different dimensions.

- **Chapter 2** Stochastic Resolvent Method: Development and Analysis of Efficient Algorithms for Estimating the Minimum Eigenvalue addresses the problem of estimating the minimum eigenvalue of symmetric square matrices using their resolvent matrix. The Resolvent Power Method and its stochastic implementations via Resolvent Monte Carlo (RMC) and Resolvent Quasi-Monte Carlo (RQMC) approaches are presented. The chapter investigates the role of parameters affecting the convergence of the infinite series representing the resolvent matrix. Almost optimal RMC and RQMC algorithms are constructed and the balance between stochastic and systematic errors is analyzed. This balance depends on the number of realizations of the random variables, the length of the Markov chain, the degree of the resolvent matrix, and the acceleration parameter included in the power series representation of the resolvent. The final section presents numerical experiments related to estimating the minimum eigenvalue of test symmetric matrices.

- **Chapter 3** Stochastic Methods for Estimating the Market Risk of Investment Portfolios is devoted to applying the algorithms developed in Chapter 1 to a real-world problem in financial mathematics: estimating the market risk of an investment portfolio. This is achieved through the maximum eigenvalue of the portfolio's correlation matrix. The largest eigenvalue is computed using the almost optimal PMC and PQMC algorithms. When applying the almost optimal PQMC algorithm, two variants are considered: (1) using scrambled Sobol and Halton sequences with default settings; (2) using scrambled Sobol and Halton sequences with the *skip* and *leap* parameters. Numerical experiments on real financial data demonstrate the applicability and efficiency of the proposed algorithms.

The concluding section includes a list of publications, approbation, scientific and applied contributions, and acknowledgements.

1. Stochastic Power Method: Development and Investigation of Efficient Algorithms for Estimating the Maximum Eigenvalue

1.1 Problem Formulation

Let $A = \{a_{ij}\}_{i,j=1}^{n} \in \mathbb{R}^{n\times n}$ be a given nonsingular symmetric matrix. The eigenvalues (spectrum) of the matrix A are defined as the real values of the parameter $\lambda(A)$ for which the equation:

$$A\mathbf{x} = \lambda(A)\mathbf{x}, \text{ where } \mathbf{x} \in \mathbb{R}^n, \tag{1.1}$$

has a nonzero solution, and the corresponding nonzero vectors $\mathbf{x}$ are called eigenvectors of A. A necessary and sufficient condition for the existence of a nonzero solution is that the parameter $\lambda(A)$ be a root of the characteristic equation $|A - \lambda(A)\mathbf{I}| = 0$, where $\mathbf{I}$ is the unit n-dimensional matrix [90].
It is assumed that the eigenvalues of A are ordered by absolute value and satisfy the inequalities:

$$\lambda_{min} = |\lambda_n| \leq |\lambda_{n-1}| \leq |\lambda_{n-2}| \leq \cdots \leq |\lambda_2| < |\lambda_1| = \lambda_{max}. \tag{1.2}$$

We consider the task of developing and investigating efficient algorithms based on the Stochastic Power method to estimate λ_{max}, which, according to (1.2), is unique.

1.2 Methods for Estimating the Largest Eigenvalue

1.2.1 Power Method

The Power method is a *classical* iterative numerical method for approximating the maximum eigenvalue $\lambda_{\max}$ of square matrices [33, 43], based on the Rayleigh quotient [43]:

$$r(\boldsymbol{x}) = \frac{\boldsymbol{x}^T A\boldsymbol{x}}{\boldsymbol{x}^T\boldsymbol{x}}.$$

The algorithm is implemented by initializating with a normalized initial vector, iteratively updating the vector and evaluating the eigenvalue after k iterations, i.e.

$$\lambda_{max} \approx \lambda_{max}^{(k)} = r(\boldsymbol{x}_k).$$

According to conditions (1.2), the obtained approximation corresponds to the dominant eigenvalue.
Systematic error: In the case of a symmetric matrix, the error of the truncation of the Power method when representing the vectors x^T and $\boldsymbol{x}$ as linear combinations of an orthonormal basis is of the order:

$$|\lambda_{max}^{(k)} - \lambda_{max}| = \mathcal{O}\Big(\Big|\frac{\lambda_2}{\lambda_1}\Big|^{2k}\Big), \tag{1.3}$$

which shows a strong dependence on the spectral distance between the first two eigenvalues [43].
Convergence: The convergence rate of the iteration process for symmetric matrices is determined by the coefficient $\left|\frac{\lambda_2}{\lambda_1}\right|^2$, and for dominant eigenvalues in the modulus, the convergence slows down and may require the application of preprocessing techniques.
Computational complexity: The computational complexity of the Power method is $\mathcal{O}(kn^2)$, where k is the number of iterations and n is the dimension of the matrix A, which makes it suitable for large but structured symmetric problems.

1.2.2 Stochastic Power Method

The stochastic Power method, studied in the dissertation, was developed by Karaivanova and Dimov [21, 22] and is a stochastic implementation of the *classical* Power method for the eigenvalue problem (1.1) under condition (1.2). The basis of the method is the representation of the largest eigenvalue as a limit of the Rayleigh quotient:

$$\lambda_{max} = \lim_{k\to\infty} \frac{(\boldsymbol{h}, A^k\boldsymbol{f})}{(\boldsymbol{h}, A^{k-1}\boldsymbol{f})}, \tag{1.4}$$

where $\mathbf{f}$ and $\mathbf{h}$ are arbitrarily chosen and normalized vectors. If k is an arbitrarily large natural number, then

$$\lambda_{max}^{(k)} = \frac{(\boldsymbol{h}, A^k \boldsymbol{f})}{(\boldsymbol{h}, A^{k-1} \boldsymbol{f})} \tag{1.5}$$

is an approximation of λ_{max} with a certain systematic error.
The stochastic Power method is implemented by constructing random variables whose mathematical expectations coincide with the scalar products in the numerator and denominator of the above relation. To estimate $(\mathbf{h}, A^k\mathbf{f})$, a random variable $\theta^{(k)}$ is defined, based on a discrete finite Markov chain with states:

$$l_0 \to \cdots \to l_t \to \cdots \to l_k \ \ (1 \le l_t \le n,\ 0 \le t \le k), \tag{1.6}$$

with an initial density vector $\boldsymbol{p} = \{p_i\}_{i=1}^n \in \mathbb{R}^n$ and a transition density matrix $P = \{p_{ij}\}_{i,j=1}^n \in \mathbb{R}^{n\times n}$. The construction involves iterative calculation of the weight W_k:

$$W_0 = 1,\ W_t = W_{t-1}\frac{a_{l_{t-1}l_t}}{p_{l_{t-1}l_t}},\ t = 1, \ldots, k, \tag{1.7}$$

and a random variable $\theta^{(k)}$ is defined by

$$\theta^{(k)} = \frac{h_{l_0}}{p_{l_0}} W_k f_{l_k}. \tag{1.8}$$

The random variable $\theta^{(k)}$ defined by (1.8) has an expectation equal to the scalar product $(\mathbf{h}, A^k\mathbf{f})$, i.e. $E[\theta^{(k)}] = (\mathbf{h}, A^k\mathbf{f})$ [17].

Definition 1.2.1. *The initial density vector $\boldsymbol{p} = \{p_i\}_{i=1}^n \in \mathbb{R}^n$ is called permissible for a vector $\boldsymbol{h} = \{h_i\}_{i=1}^n \in \mathbb{R}^n$, i.e. $\boldsymbol{p} \in \mathfrak{P}_{\boldsymbol{h}}$, if $p_i > 0$, when $h_i \neq 0$ and $p_i = 0$, when $h_i = 0$ for $i = 1, \ldots, n$.*

Definition 1.2.2. *A transition density matrix $P = \{p_{ij}\}_{i,j=1}^n \in \mathbb{R}^{n\times n}$ is called permissible for a symmetric matrix $A = \{a_{ij}\}_{i,j=1}^n \in \mathbb{R}^{n\times n}$, i.e. $P \in \mathfrak{P}_A$, if $p_{ij} > 0$, when $a_{ij} \neq 0$ and $p_{ij} = 0$, when $a_{ij} = 0$ for $i, j = 1, \ldots, n$.*

The introduced concepts of an admissible initial density vector $\mathbf{p} \in \mathfrak{P}_{\mathbf{h}}$ and an admissible transition density matrix $P \in \mathfrak{P}_A$ guarantee the correct construction of the Markov chain. For a sample of N realizations of the random variable $\theta^{(k)}$, the mean is represented by:

$$\overline{\theta}_N^{(k)} = \frac{1}{N}\sum_{s=1}^{N} (\theta^{(k)})_s, \tag{1.9}$$

where $(\theta^{(k)})_s$ denotes the s-th realization of $\theta^{(k)}$ for $1 \le s \le N$. This means provides a stochastic approximation of $(\mathbf{h}, A^k\mathbf{f})$. When pseudorandom number generators are used, this is a Monte Carlo estimate with probabilistic error:

$$R_N^{(k)} = |(\boldsymbol{h}, A^k\boldsymbol{f}) - \overline{\theta}_N^{(k)}| < c_1 \sigma(\theta^{(k)}) N^{-1/2}, \tag{1.10}$$

where c_1 is a constant and $\sigma(\theta^{(k)})$ is the standard deviation [17]. When low-discrepancy sequences (Sobol, Halton) are used, $\overline{\theta}_N^{(k)}$is a Quasi-Monte Carlo approximation with error:

$$QR_N^{(k)} = |(\boldsymbol{h}, A^k\boldsymbol{f}) - \overline{\theta}_N^{(k)}| < c_2 \frac{(\log N)^{k+1}}{N}, \tag{1.11}$$

obtained by the Koksma-Hlawka inequality, where $(k+1)$ is the dimension of the sequences used.

Theorem 1.2.1. [1] *Let $\theta^{(k)}$ and $\theta^{(k-1)}$ be random variables for fixed steps k and $k-1$ of the Markov chain (1.6). Then*

$$\frac{E[\theta^{(k)}]}{E[\theta^{(k-1)}]} = \lambda_{max}^{(k)}. \tag{1.12}$$

Remark 1. *The stochastic Power method is called the Power Monte Carlo (PMC) method when the samples for $\theta^{(k)}$ and $\theta^{(k-1)}$ are generated using random number generators to construct the Markov chain (1.6).*

In this case, the stochastic error of the PMC method is determined by the probabilistic error defined in (1.10).

[1] The proof of Theorem 1.2.1 is provided in the dissertation.

Remark 2. *When scrambled low-discrepancy sequences, such as scrambled Sobol sequences [75], are used to construct the Markov chain for generating samples of $\theta^{(k)}$ and $\theta^{(k-1)}$, the stochastic Power method is called the Power Quasi-Monte Carlo (PQMC) method.*

The stochastic error of the PQMC method is determined by the error defined in (1.11).
Reformulating the problem in terms of integral equations with appropriately chosen kernels and domains allows the use of the Koksma-Hlawka inequality when analyzing the convergence of the considered algorithms. In general, the use of low-discrepancy sequences (so-called quasi-sequences) improves the convergence rate of the corresponding QMC algorithms. Still, it does not allow for a posteriori error estimation. Scrambling (randomization) of the quasi-sequence makes it possible to overcome this drawback.
The theoretical comparison of the error in the PMC and PQMC methods shows that in both cases the error is a product of two factors: one depending on the sequence and the other on the function or the random variable. In this context, the Koksma-Hlawka inequality represents a worst-case bound, whereas the error in the PMC approach has a probabilistic nature. Moreover, computational experience shows that the variation $V(f)$ in the Koksma–Hlawka inequality is usually overestimated, while the second factor, the discrepancy of the sequence, reflects the actual order of the error.

1.3 Almost Optimal PMC and PQMC Methods and Algorithms

1.3.1 Refining the Construction of $\theta^{(k)}$ and $\theta^{(k-1)}$ with *Almost Optimal* Probabilities for the Markov Chain: Error Balancing

Let the symmetric matrix A be represented by its rows $\boldsymbol{a}_i$, introducing standard ℓ_1-norms for vectors and matrices:

$$\|\boldsymbol{h}\| = \|\boldsymbol{h}\|_1 = \sum_{i=1}^{n} |h_i|, \;\; \|\boldsymbol{a}_i\| = \|\boldsymbol{a}_i\|_1 = \sum_{j=1}^{n} |a_{ij}|, \;\; \|A\| = \|A\|_1 = \max_j \sum_{i=1}^{n} |a_{ij}|, \;\; j = 1, \ldots, n.$$

The probability error of the MC approximations, according to (1.10), depends on the standard deviation $\sigma(\theta^{(k)})$ and the number of realizations N. For a fixed N, it is determined mainly by the variance of the random variable $\theta^{(k)}$. The variance depends on the choice of the admissible initial density vector $\boldsymbol{p} \in \mathfrak{P}_{\boldsymbol{h}}$ and the transition density matrix $P \in \mathfrak{P}_A$. All such choices can be used to construct estimates for $\lambda_{max}^{(k)}$, provided that the variances are finite.
The most commonly used approach to constructing a Markov chain for linear algebra problems is based on the uniform distribution. In this case, the coordinates of the density vector $\boldsymbol{p}$ and the elements of the transition density matrix P are set equal to $\frac{1}{n}$, i.e.,

$$\boldsymbol{p} = \{p_i\}_{i=1}^{n} = \frac{1}{n} \text{ and } P = \{p_{ij}\}_{i,j=1}^{n} = \frac{1}{n}, \quad i, j = 1, \ldots, n. \tag{1.13}$$

When choice (1.13) is used to construct a Markov chain, the Power MC and Power QMC methods are called *classical*.
Appropriate choices of $\boldsymbol{p}$ and P allow the construction of more efficient algorithms, leading to a reduction in variance, a reduction in computational complexity, and greater precision compared to the *classical* case. There is an *almost optimal* choice, represented by the formulas:

$$\boldsymbol{p} = \{p_i\}_{i=1}^{n}, \;\; p_i = \frac{|h_i|}{\|\boldsymbol{h}\|} \text{ and } P = \{p_{ij}\}_{i,j=1}^{n}, \;\; p_{ij} = \frac{|a_{ij}|}{\|\boldsymbol{a}_i\|}, \;\; i, j = 1, \ldots, n. \tag{1.14}$$

This choice leads to a significant reduction in variance and the construction of the random variable $\theta^{(k)}$ differs significantly from the *classical* PMC/PQMC method.

Theorem 1.3.1. [2] *Let $\boldsymbol{p}$ and P be the almost optimal initial density vector and the almost optimal transition density matrix (see (1.14)). Then the mean value (1.9) can be expressed as follows:*

$$\overline{\theta}_N^{(k)} = \frac{1}{N} \sum_{s=1}^{N} sign(h_{l_0^{(s)}}) \|\boldsymbol{h}\| \left\{ \prod_{t=1}^{t=k} sign(a_{l_{t-1}^{(s)} l_t^{(s)}}) \|\boldsymbol{a}_{l_{t-1}^{(s)}}\| \right\} f_{l_k^{(s)}}. \tag{1.15}$$

The following corollaries follow from Theorem 1.2.1 and Theorem 1.3.1:

[2] The proof of Theorem 1.3.1 is given in the dissertation.

Corollary 1. *Let $\boldsymbol{p}$ and P be the almost optimal initial density vector and the almost optimal density matrix. Then the Stochastic Power Method for estimating $\lambda_{max}^{(k)}$ is defined as the ratio of the sample means of the random variables $\overline{\theta}_N^{(k)}$ and $\overline{\theta}_N^{(k-1)}$ given by (1.15), i.e.*

$$\lambda_{max}^{(k)} \approx \frac{\sum_{s=1}^{N} sign(h_{l_0^{(s)}}) \left\{ \prod_{t=1}^{t=k} sign(a_{l_{t-1}^{(s)} l_t^{(s)}}) \| \boldsymbol{a}_{l_{t-1}^{(s)}} \| \right\} f_{l_k^{(s)}}}{\sum_{s=1}^{N} sign(h_{l_0^{(s)}}) \left\{ \prod_{t=1}^{t=k-1} sign(a_{l_{t-1}^{(s)} l_t^{(s)}}) \| \boldsymbol{a}_{l_{t-1}^{(s)}} \| \right\} f_{l_{k-1}^{(s)}}}. \tag{1.16}$$

Corollary 2. *Assume that the L_1-norm of all row vectors of the symmetric matrix A is equal to a constant a, i.e.*

$$\|\boldsymbol{a}_i\|_1 = \|\boldsymbol{a}_i\| = \sum_{j=1}^{n} |a_{ij}| = a, \;\; i = 1, \ldots, n. \tag{1.17}$$

Then the estimator of $\lambda_{max}^{(k)}$ given by (1.16) can be rewritten in a simpler form:

$$\lambda_{max}^{(k)} \approx \frac{\sum_{s=1}^{N} sign(h_{l_0^{(s)}}) \left\{ \prod_{t=1}^{t=k} sign(a_{l_{t-1}^{(s)} l_t^{(s)}}) \right\} a \, f_{l_k^{(s)}}}{\sum_{s=1}^{N} sign(h_{l_0^{(s)}}) \left\{ \prod_{t=1}^{t=k-1} sign(a_{l_{t-1}^{(s)} l_t^{(s)}}) \right\} f_{l_{k-1}^{(s)}}}. \tag{1.18}$$

Corollary 3. *Let the L_1-norm of all row vectors of the symmetric matrix A satisfy condition (1.17). Assume that the following condition holds for all elements of A:*

$$sign(h_{l_0^{(s)}}) \prod_{t=1}^{t=k-1} sign(a_{l_{t-1}^{(s)} l_t^{(s)}}) = 1, \;\; s = 1, \ldots, N. \tag{1.19}$$

Then $\lambda_{max}^{(k)}$ can be estimated by an even simpler formula:

$$\lambda_{max}^{(k)} \approx \frac{\sum_{s=1}^{N} sign(a_{l_{k-1}^{(s)} l_k^{(s)}}) \, a \, f_{l_k^{(s)}}}{\sum_{s=1}^{N} f_{l_{k-1}^{(s)}}}. \tag{1.20}$$

It should be noted that by Corollary (2) and Corollary (3) simplified estimates are constructed for an approximate calculation of $\lambda_{max}^{(k)}$ for certain classes of symmetric matrices. According to Remark 3, these classes are nonempty sets.

Remark 3. *The set of symmetric matrices that satisfy the conditions of Corollary 3 is nonempty. For example, consider a symmetric matrix A with positive entries, for which all diagonal elements are equal, i.e., $a_{ii} = b > 0, \;\; i = 1, \ldots, n$, and all off-diagonal elements are also equal, i.e., $a_{ij} = d > 0, \;\; i \neq j, \;\; i, j = 1, \ldots, n$.*

Since the systematic error ε_1 depends on the number k of transitions in the Markov chain, and the stochastic error ε_2 depends on the number of realizations N, an estimate of the corresponding errors is obtained:

$$|\lambda_{max} - \frac{\overline{\theta}_N^{(k)}}{\overline{\theta}_N^{(k-1)}}| = |\lambda_{max} - \lambda_{max}^{(k)} + \lambda_{max}^{(k)} - \frac{\overline{\theta}_N^{(k)}}{\overline{\theta}_N^{(k-1)}}| \leq |\lambda_{max} - \lambda_{max}^{(k)}| + |\lambda_{max}^{(k)} - \frac{\overline{\theta}_N^{(k)}}{\overline{\theta}_N^{(k-1)}}| < \epsilon_1 + \epsilon_2. \tag{1.21}$$

An optimal balance between the two types of errors (systematic and stochastic) is achieved when $\epsilon_1 = \epsilon_2 = \epsilon$.

Definition 1.3.1. *PMC and PQMC methods for estimating the maximum eigenvalue of a symmetric matrix, with the choice of the initial density vector $\boldsymbol{p}$ and the transition density matrix P according to equation (1.14), are referred to as almost optimal PMC and PQMC methods.*

1.3.2 Almost Optimal PMC and Almost Optimal PQMC Algorithms: Computational Complexity

The pseudocode in **Algorithm 1** describes a procedure to estimate the maximum eigenvalue of a dense symmetric matrix based on formula (1.16) and Corollary 1. The algorithm is defined as an *almost optimal* PQMC algorithm when low-discrepancy sequences (Sobol or Halton) are used in Step 4 and as an *almost optimal* PMC algorithm, indicated by **Algorithm (1a)**, when pseudorandom number generators are used. If the conditions

of Corollary 2 and Corollary 3 are satisfied, the formulas in Step 6 can be replaced by the simpler expressions (1.18) or (1.20).

Algorithm 1 Pseudocode for computing the *Almost Optimal* PQMC algorithm

1: INPUT: matrix $A = \{a_{ij}\} \in \mathbb{R}^{n\times n}$; vectors $\boldsymbol{h}, \boldsymbol{f} \in \mathbb{R}^n$ and positive integers n, N, k

2: COMPUTE: $\|\boldsymbol{a}_i\| = \sum_{j=1}^{n} |a_{ij}|, \quad 1 \le i \le n \quad \text{and} \quad \|\boldsymbol{h}\| = \sum_{i=1}^{n} |h_i|$

3: COMPUTE: The coordinates of a permissible density vector $\boldsymbol{p}$ and the elements of a permissible density matrix P

$$p_i = \frac{|h_i|}{\|\boldsymbol{h}\|} \quad \text{and} \quad p_{ij} = \frac{|a_{ij}|}{\|\boldsymbol{a}_i\|}, \ i, j = 1, \ldots, n.$$

4: GENERATE: N elements of the $(k+1)$ - dimensional Sobol (or Halton) sequence

5: CONSTRUCT: N realizations of the Markov chain with integer elements

$$l_0^{(s)} \to \ldots \to l_t^{(s)} \to \ldots \to l_{k-1}^{(s)} \to \ l_k^{(s)}, \ 1 \le l_t^{(s)} \le n, \ 0 \le t \le k, \ 1 \le s \le N$$

6: COMPUTE:

$$\overline{\theta}_N^{(k)} = \frac{1}{N} \sum_{s=1}^{N} sign(h_{l_0^{(s)}}) \|\boldsymbol{h}\| \{ \prod_{t=1}^{t=k} sign(a_{l_{t-1}^{(s)} l_t^{(s)}}) \|\boldsymbol{a}_{l_{t-1}^{(s)}}\| \} f_{l_k^{(s)}};$$

$$\overline{\theta}_N^{(k-1)} = \frac{1}{N} \sum_{s=1}^{N} sign(h_{l_0^{(s)}}) \|\boldsymbol{h}\| \{ \prod_{t=1}^{t=k-1} sign(a_{l_{t-1}^{(s)} l_t^{(s)}}) \|\boldsymbol{a}_{l_{t-1}^{(s)}}\| \} f_{l_{k-1}^{(s)}};$$

7: OUTPUT:

$$\lambda_{max}^{(k)} := \frac{\overline{\theta}_N^{(k)}}{\overline{\theta}_N^{(k-1)}}$$

The computational complexity of **Algorithm 1** is determined by the number of realizations N of the Markov chain, the average time required to compute a single realization of the random variables $\theta^{(k)}$ and $\theta^{(k-1)}$, and the preprocessing cost associated with the construction of the transition density matrix P. Steps 2 and 3 require $\mathcal{O}(n^2)$ operations and are treated as preprocessing, while the main computational effort is concentrated in Steps 4 to 6. For fixed k, the time for a single realization is $\tau_k = \mathcal{O}(nk)$; therefore, the total computational complexity of the algorithm is:

$$Cost(Alg1) = \mathcal{O}(Nnk) + \mathcal{O}(n^2) = \mathcal{O}(Nnk + n^2),$$

which reduces to $\mathcal{O}(Nnk)$ when $N > n$. Numerical experiments show that for dense symmetric matrices, a balance between systematic and stochastic errors is achieved for $N = \mathcal{O}(n)$, while for sparse matrices, an additional reduction in computational cost can be expected.

1.4 Numerical Results and Discussion

In the numerical experiments, the *almost optimal* PMC algorithm (**Algorithm (1a)**) is implemented using two pseudorandom number generators: Mersenne Twister (MT) and Middle Square (MS). The corresponding implementations are denoted by $PMC_{(MT)}$ and $PMC_{(MS)}$. The results obtained are compared with those of the *classical* PMC algorithm, implemented using the standard choice of the initial density vector and the transition density matrix according to formula (1.14), denoted by $PMC_{(MT)}^{(n)}$ and $PMC_{(MS)}^{(n)}$. The *almost optimal* PQMC algorithm (**Algorithm 1**) is implemented using low-discrepancy sequences (Sobol and Halton) denoted by $PQMC_{(S)}$ and $PQMC_{(H)}$, and is compared with the *classical* PQMC approach and its variants $PQMC_{(S)}^{(n)}$ and $PQMC_{(H)}^{(n)}$. To reduce correlations in high dimensions, the sequences are scrambled using "RR2" (reverse-radix) for Halton and "MatousekAffineOwen" for Sobol. All generators and sequences are implemented in MATLAB 9.10 (R2021a).

The numerical experiments are carried out on two symmetric dense matrices of sizes $n = 100$ and $n = 500$, with randomly generated entries and eigenvalues $(\lambda_1, \lambda_2) = (50.0408, 4.0522)$ and $(\lambda_1, \lambda_2) = (250.2454, 9.0721)$ respectively. The vectors $\boldsymbol{h}$ and $\boldsymbol{f}$ are chosen to have unit norm L_1. To ensure convergence, the matrix A is scaled by the parameter q as:

$$q = \frac{1}{|\lambda_1| + \delta_1}, \ \delta_1 > 0,$$

or alternatively

$$q = \frac{1}{\max_i \|\boldsymbol{a}_i\| + \delta}, \;\; \delta > 0, \;\; i = 1, \ldots, n,$$

where $\|\boldsymbol{a}_i\|$ denotes the L_1-norm of the i-th row of A. The choice of well-separated eigenvalues guarantees fast convergence and allows for an experimental investigation of the balance between systematic and stochastic errors. The influence of the number of transitions k and the number of realizations N on accuracy is analyzed, as well as the effect of variance reduction achieved by the *almost optimal* PMC/PQMC algorithms under fixed computational complexity.

1.4.1 Case (i): Matrix size $n = 100$

Table 1.1 presents the results for estimating the largest eigenvalue of a symmetric matrix ($n = 100$, $\lambda_1 = 50.0408$) using the *almost optimal* $PMC_{(MT)}$ and the *classical* $PMC^{(n)}_{(MT)}$ algorithm. The optimal balance between systematic and stochastic error is achieved for $k = 8$ and $k = 9$. The minimum absolute error for $PMC_{(MT)}$ is 5×10^{-5} at $k = 8, N = 512$, whereas for the *classical* $PMC^{(n)}_{(MT)}$ an error of 1.5×10^{-3} is observed in $k = 8, N = 2048$. This clearly demonstrates the superiority of the almost optimal variant.

Table 1.1: Results of $PMC_{(MT)}$ and $PMC^{(n)}_{(MT)}$ at different N and k for a matrix A with size $n = 100$, for which $\lambda_2/\lambda_1 \approx 0.081$, where $\lambda_1 = 50.0408$ and $\lambda_2 = 4.0522$.

N	**k**	$\lambda_1^{(k)}$ **using** $\mathrm{PMC}_{(\mathrm{MT})}$	**Absolute Error** $\mathrm{PMC}_{(\mathrm{MT})}$	$\lambda_1^{(k)}$ **using** $\mathrm{PMC}^{(\mathrm{n})}_{(\mathrm{MT})}$	**Absolute Error** $\mathrm{PMC}^{(\mathrm{n})}_{(\mathrm{MT})}$
128	8	50.039901	0.00090	50.019883	0.0209
	9	**50.040709**	**0.00009**	**50.037795**	**0.0030**
	10	50.045295	0.00450	50.066104	0.0253
256	7	50.023923	0.01688	50.012158	0.0286
	8	**50.040628**	**0.00017**	**50.039528**	**0.0013**
	9	50.044896	0.00410	50.050593	0.0098
512	7	50.035045	0.00576	49.996040	0.0448
	8	**50.040750**	**0.00005**	**50.039264**	**0.0015**
	9	50.052027	0.01123	50.050158	0.0094
1024	7	50.029828	0.01097	50.019435	0.0214
	8	**50.040720**	**0.00008**	**50.039735**	**0.0011**
	9	50.045403	0.00460	50.054351	0.0136
2048	7	50.036291	0.00451	50.029563	0.0112
	8	**50.041086**	**0.00029**	**50.041728**	**0.0009**
	9	50.043850	0.00305	50.057179	0.0164

*The highlighted rows represent the optimal k values for each N.

Table 1.2 shows the analogous results for $PMC_{(MS)}$ and $PMC^{(n)}_{(MS)}$. The smallest absolute error for the *almost optimal* MS algorithm is 1.8×10^{-4} in $k = 8$ and $N = 512$, while the *classical* MS algorithm reaches an error of 1.8×10^{-3}. This confirms the general trend that *almost optimal* algorithms reduce variance and yield more accurate estimates than *classical* ones, regardless of the pseudorandom number generator used.
Figure 1.1 shows that the *almost optimal* versions ($PMC_{(MT)}$ and $PMC_{(MS)}$) follow uniform trajectories close to the exact value λ_{max} even for smaller values of N, while the *classical* versions, especially $PMC^{(n)}_{(MS)}$, demonstrate larger fluctuations and weaker stability. The main reason is the reduced variance in the construction of random variables $\theta^{(k)}$ and $\theta^{(k-1)}$ using the optimal transition density matrix, which confirms the higher precision and computational efficiency of the *almost optimal* PMC algorithms.
Table 1.3 presents the results for the *almost optimal* and *classical* PQMC algorithms based on Halton sequences, when evaluating $\lambda_1 = 50.0408$ for a matrix of size $n = 100$. A monotonic decrease in absolute error is observed as the number of transitions k increases, with optimal convergence achieved at $k = 11$-12. For $N = 2048$, the algorithm $PQMC_{(H)}$ reaches an absolute error of 8.2×10^{-4}, while the *classical* $PQMC^{(n)}_{(H)}$ remains significantly less accurate with an error of 0.0707. This clearly demonstrates the advantage of the *almost optimal* construction.
Table 1.4 contains the analogous results for the algorithms based on Sobol sequences. The *almost optimal* algorithm $PQMC_{(S)}$ systematically outperforms both its *classical* counterpart and the variant based on Halton sequences. For example, for $N = 2048$ and an optimal number of transitions, $PQMC_{(S)}$ achieves an absolute error of 5×10^{-5}, while $PQMC^{(n)}_{(S)}$ reaches 0.0336. Even for smaller values of N, such as $N = 256$ and $k = 11$, the difference is significant: 8.1×10^{-4} versus 0.1455 in favor of the *almost optimal* algorithm.

Table 1.2: Results of $PMC_{(MS)}$ and $PMC^{(n)}_{(MS)}$ at different N and k for the matrix A with size $n = 100$, for which $\lambda_2/\lambda_1 \approx 0.081$, where $\lambda_1 = 50.0408$ and $\lambda_2 = 4.0522$.

N	k	$\lambda_1^{(k)}$ using $\mathrm{PMC}_{(\mathrm{MS})}$	Absolute Error $\mathrm{PMC}_{(\mathrm{MS})}$	$\lambda_1^{(k)}$ using $\mathrm{PMC}^{(\mathrm{n})}_{(\mathrm{MS})}$	Absolute Error $\mathrm{PMC}^{(\mathrm{n})}_{(\mathrm{MS})}$
	8	50.039440	0.00136	50.019388	0.0214
128	**9**	**50.040595**	**0.00020**	**50.029883**	**0.0109**
	10	50.051262	0.01046	50.060923	0.0201
	7	50.031044	0.00976	49.984883	0.0559
256	**8**	**50.042490**	**0.00169**	**50.028211**	**0.0126**
	9	50.050490	0.00969	50.051251	0.0105
	7	50.030518	0.01028	49.997989	0.0428
512	**8**	**50.040617**	**0.00018**	**50.033570**	**0.0072**
	9	50.058913	0.01811	50.053570	0.0128
	10	50.061048	0.02025	50.091035	0.0502
	7	50.031472	0.00933	50.009835	0.0310
1024	**8**	**50.041209**	**0.00041**	**50.038850**	**0.0020**
	9	50.044938	0.00414	50.056396	0.0156
	7	50.038998	0.00180	50.022658	0.0181
2048	**8**	**50.041243**	**0.00044**	**50.038951**	**0.0018**
	9	50.043045	0.00225	50.063537	0.0227

*The highlighted rows represent the optimal k values for each N.

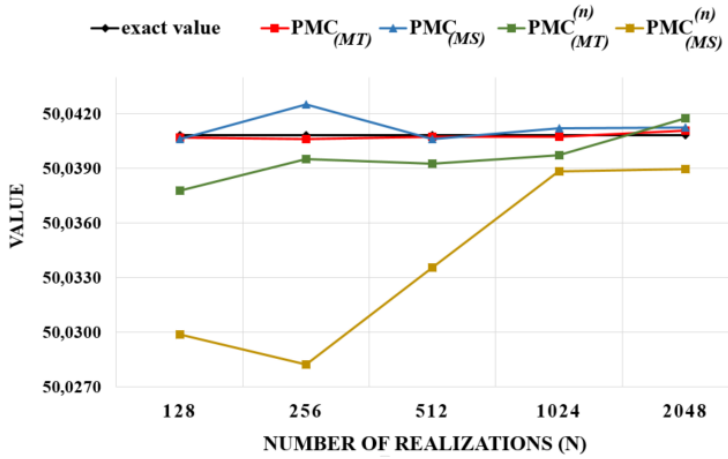


Figure 1.1: Comparison of the approximate results for $\lambda_{max}^{(k)}$ with $\lambda_{max} = 50.0408$ in the balanced error case, i.e. when $(k = 9, N = 128)$ and $(k = 8, N > 128)$. Applied algorithms: $PMC_{(MT)}$, $PMC_{(MS)}$, $PMC^{(n)}_{(MT)}$ and $PMC^{(n)}_{(MS)}$.

The visualization in Figure 1.2 confirms the tabular results, showing a smoother and more stable convergence of the algorithms $PQMC_{(S)}$ and $PQMC_{(H)}$ toward the exact value λ_{max} for all values of N. In contrast, the *classical* variants $PQMC^{(n)}_{(S)}$ and $PQMC^{(n)}_{(H)}$ demonstrate larger fluctuations and initial overestimation of the eigenvalue, and their convergence is significantly slower.
Figure 1.3 shows a comparison between the *almost optimal* PMC and PQMC algorithms for the balanced cases. In PMC methods, $PMC_{(MT)}$ reaches a minimum error of 5×10^{-5} at $N = 512$ and $k = 8$, while $PMC_{(MS)}$ shows a larger but still small error of 1.8×10^{-4}. On the PQMC side, $PQMC_{(S)}$ is the most accurate, with an error of 5×10^{-5} at $N = 2048$ and $k = 11$, while $PQMC_{(H)}$ reaches 8.2×10^{-4}. These results clearly show that the use of scrambled Sobol sequences and the *almost optimal* transition matrix leads to lower variance and an optimal balance between stochastic and systematic error compared to their *classical* variants.

1.4.2 Case (ii): Matrix size $n = 500$

Table 1.5 presents the results for estimating the maximum eigenvalue λ_{max} of a symmetric dense matrix of size $n = 500$, obtained with the *almost optimal* algorithm $PMC_{(MT)}$ and its *classical* analogue $PMC^{(n)}_{(MT)}$. Numerical data show that for a fixed number of realizations N, increasing the number of transitions k leads to a decrease in the absolute error, with the optimal balance between systematic and stochastic error being

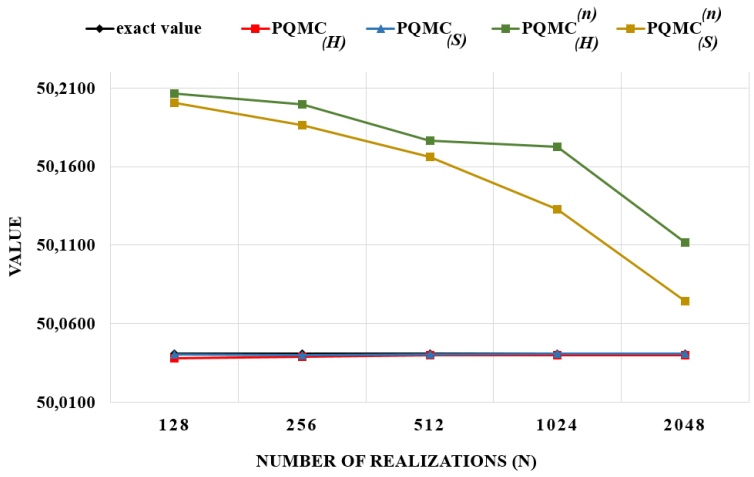


Figure 1.2: Comparison of the approximate results for $\lambda_{max}^{(k)}$ with $\lambda_{max} = 50.0408$ in the balanced error case, i.e. when $(k = 12, N = 128)$ and $(k = 11, N > 128)$. Applied algorithms: $PQMC_{(S)}$, $PQMC_{(H)}$, $PQMC_{(S)}^{(n)}$ and $PQMC_{(H)}^{(n)}$.

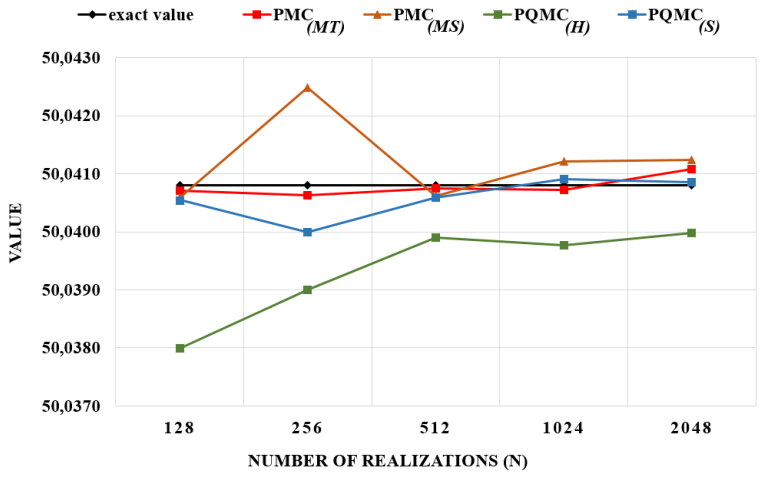


Figure 1.3: Comparison of λ_{max} of the symmetric matrix A $(n = 100)$ with $\lambda_{max}^{(k)}$ in the balancing cases. The *almost optimal* PMC and PQMC algorithms are used.

achieved at $k = 9$. In this balanced case, the *almost optimal* algorithm reaches an absolute error of the order of 10^{-4} (e.g., for $N = 512$), while in the *classical* variant the error remains of the order of 10^{-2} under the same parameters, clearly demonstrating significantly higher accuracy.

Similar conclusions can be drawn from Table 1.6, which presents the results for the *almost optimal* algorithm $PMC_{(MS)}$ and the *classical* $PMC_{(MS)}^{(n)}$. In this case, optimal convergence is observed at $k = 9$, with the minimum absolute error for the *almost optimal* algorithm achieved at $N = 128$ on the order of 10^{-4}. In contrast, the *classical* variant demonstrates significantly larger errors, on the order of 10^{-2}, which confirms the advantage of the optimized design even when using a weaker pseudorandom generator.

The visualization in Figure 1.4 confirms the results in Table 1.5 and Table 1.6. The *almost optimal* PMC algorithms show smoother and more stable convergence to λ_{max} with increasing number of realizations N. This is due to the significantly reduced variance in the construction of the random variables $\theta^{(k)}$ and $\theta^{(k-1)}$. The *classical* algorithm $PMC_{(MS)}^{(n)}$ demonstrates fluctuations and even overestimation of the eigenvalue at larger values of N, while $PMC_{(MT)}^{(n)}$ is characterized by more stable convergence. This indicates that the MT pseudorandom number generator is preferable for high-dimensional problems.

Table 1.7 presents the results for estimating λ_{max} using the *almost optimal* and *classical* PQMC algorithms based on scrambled Halton sequences. For all algorithms, the absolute error decreases as the number of transitions k increases, with the optimal balance achieved at $k = 12$. In this case, the *almost optimal* algorithm $PQMC_{(H)}$ achieves an absolute error on the order of 10^{-3} (e.g., 4.59×10^{-3} at $N = 2048$), while the *classical* variant $PQMC_{(H)}^{(n)}$ demonstrates significantly larger errors, reaching 0.0726 for the same number of realizations. This

Table 1.3: Results of $PQMC_{(H)}$ and $PQMC_{(H)}^{(n)}$ for different N and k for a matrix A with size $n = 100$, for which $\lambda_2/\lambda_1 \approx 0.081$, where $\lambda_1 = 50.0408$ and $\lambda_2 = 4.0522$.

N	**k**	$\lambda_1^{(k)}$ **using** $\mathrm{PQMC_{(H)}}$	**Absolute Error** $\mathrm{PQMC_{(H)}}$	$\lambda_1^{(k)}$ **using** $\mathrm{PQMC_{(H)}^{(n)}}$	**Absolute Error** $\mathrm{PQMC_{(H)}^{(n)}}$
128	11	49.801798	0.23900	49.574856	0.4659
	12	**50.037989**	**0.00281**	**50.206208**	**0.1654**
	13	50.152986	0.11219	50.314121	0.2733
256	10	50.001834	0.03897	49.739820	0.3010
	11	**50.038996**	**0.00180**	**50.199525**	**0.1587**
	12	50.067986	0.02719	50.229280	0.1885
512	10	50.017989	0.02281	49.749688	0.2911
	11	**50.039899**	**0.00090**	**50.176724**	**0.1359**
	12	50.178512	0.13771	50.196566	0.1558
1024	10	49.976987	0.06381	49.806135	0.2347
	11	**50.039772**	**0.00103**	**50.172345**	**0.1315**
	12	50.107985	0.06719	50.295866	0.2551
2048	10	49.973344	0.06746	49.907160	0.1336
	11	**50.039982**	**0.00082**	**50.111519**	**0.0707**
	12	50.183245	0.14245	50.275169	0.2344

*The highlighted rows represent the optimal k values for each N.

Table 1.4: Results of $PQMC_{(S)}$ and $PQMC_{(S)}^{(n)}$ for different N and k for a matrix A with size $n = 100$, for which $\lambda_2/\lambda_1 \approx 0.081$, where $\lambda_1 = 50.0408$ and $\lambda_2 = 4.0522$.

N	**k**	$\lambda_1^{(k)}$ **using** $\mathrm{PQMC_{(S)}}$	**Absolute Error** $\mathrm{PQMC_{(S)}}$	$\lambda_1^{(k)}$ **using** $\mathrm{PQMC_{(S)}^{(n)}}$	**Absolute Error** $\mathrm{PQMC_{(S)}^{(n)}}$
128	11	49.679383	0.36142	49.624160	0.4166
	12	**50.040544**	**0.00026**	**50.200481**	**0.1597**
	13	50.091116	0.05032	50.299826	0.2590
256	10	49.994318	0.04648	49.742961	0.2978
	11	**50.039989**	**0.00081**	**50.186264**	**0.1455**
	12	50.049407	0.00861	50.225854	0.1851
512	10	50.050000	0.00920	49.866152	0.1746
	11	**50.040585**	**0.00021**	**50.166400**	**0.1256**
	12	50.148019	0.10722	50.223877	0.1831
1024	10	49.986946	0.05385	49.933245	0.1076
	11	**50.040913**	**0.00011**	**50.132603**	**0.0918**
	12	50.087435	0.04664	50.167252	0.1265
2048	10	49.972883	0.06792	49.957605	0.0832
	11	**50.040854**	**0.00005**	**50.074364**	**0.0336**
	12	50.155992	0.11519	50.186986	0.1462

*The highlighted rows represent the optimal k values for each N.

clearly shows the advantage of the optimized construction of the algorithm.
Table 1.8 presents similar results for algorithms using Sobol sequences. The *almost optimal* algorithm $PQMC_{(S)}$ demonstrates the highest accuracy, with the absolute error in the balanced case at $k = 12$ on the order of 10^{-4} (e.g. 5.4×10^{-4} at $N = 2048$). In contrast, the *classical* variant $PQMC_{(S)}^{(n)}$ achieves significantly larger deviations, with an error of 0.3172 at $N = 256$. This confirms the better uniformity of Sobol sequences and their advantage in higher-dimensional problems.
Figure 1.6 shows the comparisons between the *almost optimal* PMC and PQMC algorithms. The *almost optimal* PMC algorithms $PMC_{(MT)}$ and $PMC_{(MS)}$ achieve minimum errors of 3.8×10^{-4} and 6.5×10^{-4}, respectively, at $N = 1024$ and $k = 9$, while the *almost optimal* PQMC algorithm $PQMC_{(S)}$ provides a comparable or higher accuracy at $k = 12$.
Table 1.9 compares the empirical estimates for the variances of the random variable $\theta^{(k)}$ for the *classical* and *almost optimal* PMC algorithms. Estimates were performed for matrices of dimensions $n = 100$ and $n = 500$. The results show that for the *almost optimal* PMC algorithms, the variance is about two orders of magnitude smaller compared to their *classical* variants. This estimate does not depend significantly on the generator used or on the number of realizations N, which is in agreement with the theoretical results. The fact that the variance

Table 1.5: Results of $PMC_{(MT)}$ and $PMC^{(n)}_{(MT)}$ for different N and k for a matrix A with size $n = 500$, for which $\lambda_2/\lambda_1 \approx 0.0363$, where $\lambda_1 = 250.2454$ and $\lambda_2 = 9.0721$.

N	k	$\lambda_1^{(k)}$ using $\mathrm{PMC}_{(\mathrm{MT})}$	Absolute Error $\mathrm{PMC}_{(\mathrm{MT})}$	$\lambda_1^{(k)}$ using $\mathrm{PMC}^{(\mathrm{n})}_{(\mathrm{MT})}$	Absolute Error $\mathrm{PMC}^{(\mathrm{n})}_{(\mathrm{MT})}$
128	8	250.222396	0.02300	249.492834	0.7526
	9	**250.232288**	**0.01311**	250.032970	0.2124
	10	250.295027	0.04963	**250.149293**	**0.0961**
256	8	250.228998	0.01640	250.124994	0.1204
	9	**250.250130**	**0.00473**	**250.222275**	**0.0231**
	10	250.283657	0.03826	250.311181	0.0658
512	8	250.235302	0.01011	250.115109	0.1303
	9	**250.245110**	**0.00029**	**250.192305**	**0.0531**
	10	250.268302	0.02290	250.328365	0.0830
1024	8	250.235306	0.01009	250.164200	0.0812
	9	**250.245015**	**0.00038**	**250.205542**	**0.0399**
	10	250.269913	0.02451	250.300328	0.0549
2048	8	250.226172	0.01923	250.175939	0.0695
	9	**250.246938**	**0.00154**	**250.224397**	**0.0210**
	10	250.251779	0.00638	250.295497	0.0501

*The highlighted rows represent the optimal k values for each N.

Table 1.6: Results of $PMC_{(MS)}$ and $PMC^{(n)}_{(MS)}$ at different N and k for a matrix A with size $n = 500$, for which $\lambda_2/\lambda_1 \approx 0.0363$, where $\lambda_1 = 250.2454$ and $\lambda_2 = 9.0721$.

N	k	$\lambda_1^{(k)}$ using $\mathrm{PMC}_{(\mathrm{MS})}$	Absolute Error $\mathrm{PMC}_{(\mathrm{MS})}$	$\lambda_1^{(k)}$ using $\mathrm{PMC}^{(\mathrm{n})}_{(\mathrm{MS})}$	Absolute Error $\mathrm{PMC}^{(\mathrm{n})}_{(\mathrm{MS})}$
128	8	250.211445	0.03395	249.462722	0.7827
	9	**250.245247**	**0.00015**	**250.003068**	**0.2423**
	10	250.279476	0.03408	250.120230	0.1252
256	8	250.203720	0.04168	250.015811	0.2296
	9	**250.252044**	**0.00664**	**250.221130**	**0.0243**
	10	250.290513	0.04511	250.363882	0.1185
512	8	250.206884	0.03852	250.058060	0.1873
	9	**250.244890**	**0.00051**	**250.183410**	**0.0620**
	10	250.283279	0.03788	250.356760	0.1114
1024	8	250.238977	0.00642	250.143770	0.1016
	9	**250.244751**	**0.00065**	**250.268955**	**0.0236**
	10	250.270855	0.02546	250.396782	0.1514
2048	8	250.237612	0.00779	250.103221	0.1422
	9	**250.247710**	**0.00231**	**250.320873**	**0.0755**
	10	250.275206	0.02981	250.347819	0.1024

*The highlighted rows represent the optimal k values for each N.

for the *almost optimal* versions is two orders of magnitude smaller than the *classical* versions confirms again the conclusions that these algorithms provide a more accurate estimation of the maximum eigenvalue of symmetric matrices with reduced computational complexity.

1.5 Summary

This chapter investigates the efficiency of the *almost optimal* PMC and PQMC algorithms for estimating the largest eigenvalue of dense symmetric matrices for $n = 100$ and $n = 500$. Numerical experiments show that the optimized algorithms significantly outperform the *classical* ones in accuracy and computational complexity by purposefully choosing the transition matrix and balancing systematic and stochastic error. In PMC algorithms, the optimal number of transitions is $k = 8$ for $n = 100$ and $k = 9$ for $n = 500$, with the Mersenne Twister (MT) generator providing a smaller variance than the Middle Square (MS). In the PQMC, the optimal number of transitions is $k = 11$ for $n = 100$ and $k = 12$ for $n = 500$, with the scrambled Sobol sequences leading to smoother convergence and smaller errors than Halton. Absolute errors in *almost optimal* algorithms are on the order of 10^{-4}, while in *classical* ones they reach 10^{-2}, confirming the significant reduction in variance and the

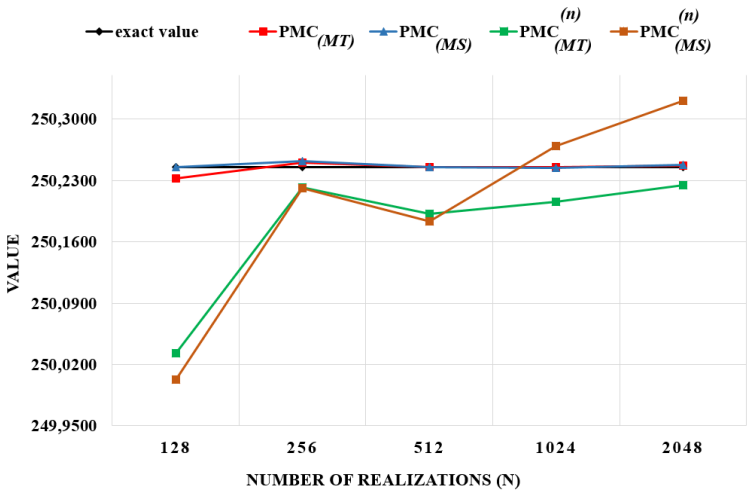


Figure 1.4: Comparison of λ_{max} for the matrix A ($n = 500$) with the approximate results for $\lambda_{max}^{(k)}$ obtained in the balanced error case, i.e. when ($k = 9, N \geq 128$). Applied algorithms: $PMC_{(MT)}$, $PMC_{(MS)}$, $PMC_{(MT)}^{(n)}$ and $PMC_{(MS)}^{(n)}$.

Table 1.7: Results of $PQMC_{(H)}$ and $PQMC_{(H)}^{(n)}$ for different N and k for matrix A with size $n = 500$. The absolute error is for the case $\lambda_2/\lambda_1 \approx 0.0363$.

N	**k**	$\lambda_1^{(k)}$ **using** $\mathrm{PQMC_{(H)}}$	**Absolute Error** $\mathrm{PQMC_{(H)}}$	$\lambda_1^{(k)}$ **using** $\mathrm{PQMC_{(H)}^{(n)}}$	**Absolute Error** $\mathrm{PQMC_{(H)}^{(n)}}$
128	11	250.167707	0.07769	251.486594	1.2412
	12	**250.249391**	**0.00399**	**249.309133**	**0.9363**
	13	250.357823	0.11242	251.999063	1.7537
256	11	250.197841	0.04756	249.470953	0.7744
	12	**250.239655**	**0.00574**	**250.770441**	**0.5250**
	13	250.357573	0.11217	251.711421	1.4660
512	11	250.089218	0.15618	249.591525	0.6539
	12	**250.236033**	**0.00937**	**250.669970**	**0.4246**
	13	250.369509	0.12411	250.978674	0.7333
1024	11	250.127756	0.11764	249.672942	0.5725
	12	**250.250718**	**0.00532**	**250.090116**	**0.1553**
	13	250.387049	0.14165	250.829267	0.5839
2048	11	250.166549	0.07885	249.987224	0.2582
	12	**250.249986**	**0.00459**	**250.172833**	**0.0726**
	13	250.321274	0.07587	250.581459	0.3361

*The highlighted rows represent the optimal k values for each N.

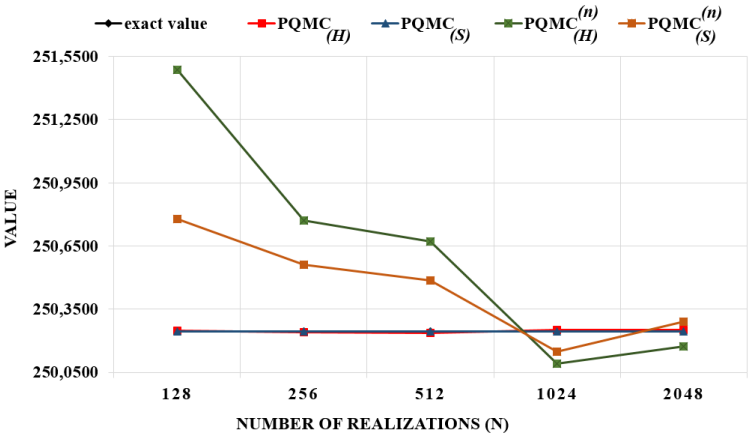


Figure 1.5: Comparison of λ_{max} for the matrix A ($n = 500$) with the approximate results for $\lambda_{max}^{(k)}$ obtained in the balanced error case, i.e. when ($k = 12, N \geq 128$). Applied algorithms: $PQMC_{(S)}$, $PQMC_{(H)}$, $PQMC_{(S)}^{(n)}$ and $PQMC_{(H)}^{(n)}$.

Table 1.8: Results of $PQMC_{(S)}$ and $PQMC_{(S)}^{(n)}$ for different N and k for matrix A with size $n = 500$. The absolute error is for the case $\lambda_2/\lambda_1 \approx 0.0363$.

N	**k**	$\lambda_1^{(k)}$ **using** $\mathrm{PQMC_{(S)}}$	**Absolute Error** $\mathrm{PQMC_{(S)}}$	$\lambda_1^{(k)}$ **using** $\mathrm{PQMC_{(S)}^{(n)}}$	**Absolute Error** $\mathrm{PQMC_{(S)}^{(n)}}$
128	11	250.236415	0.00898	249.415659	0.8297
	12	**250.245037**	**0.00036**	**250.777310**	**0.5319**
	13	250.330000	0.08460	250.989461	0.7441
256	11	250.199189	0.04621	249.483392	0.7620
	12	**250.245119**	**0.00028**	**250.562622**	**0.3172**
	13	250.291367	0.04597	250.704555	0.4592
512	11	250.099484	0.14592	249.632500	0.6129
	12	**250.244872**	**0.00053**	**250.486175**	**0.2408**
	13	250.378047	0.13265	250.679597	0.4342
1024	11	250.140000	0.10540	249.811533	0.4339
	12	**250.244996**	**0.00040**	**250.148126**	**0.0973**
	13	250.351139	0.10574	250.651883	0.4065
2048	11	250.193656	0.05174	249.937040	0.3084
	12	**250.245937**	**0.00054**	**250.290864**	**0.0455**
	13	250.272562	0.02716	250.555662	0.3103

*The highlighted rows represent the optimal k values for each N.

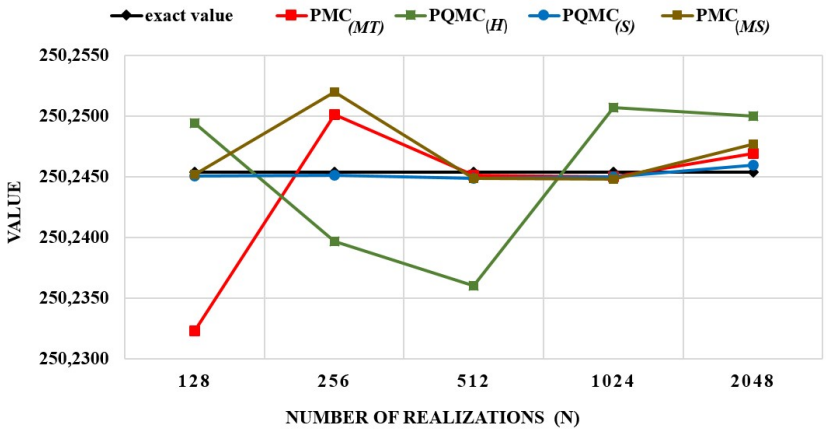


Figure 1.6: Comparison of λ_{max} of the symmetric matrix A ($n = 500$) with $\lambda_{max}^{(k)}$ in the balancing cases. The *almost optimal* PMC and PQMC algorithms are used.

Table 1.9: Variance of the maximum eigenvalue estimates for the *almost optimal* and *classical* PMC algorithms for different matrix dimensions, number of realizations (N), number of transitions (k), and the pseudorandom number generators used (MT and MS).

matrix size	N	k	$Var(PMC_{(MT)})$	$Var(PMC_{(MT)}^{(n)})$	$Var(PMC_{(MS)})$	$Var(PMC_{(MS)}^{(n)})$
100	512	8	1.169203e-06	1.720495e-04	1.236100e-06	1.781005e-04
	2048	8	1.300635e-06	1.772653e-04	1.326996e-06	1.792424e-04
500	512	9	1.186151e-08	1.229778e-05	1.269925e-08	1.285468e-05
	2048	9	1.189763e-08	1.184918e-05	1.268721e-08	1.299595e-05

increase in accuracy.

In conclusion, the *almost optimal* PMC and PQMC algorithms achieve higher accuracy with the same computational complexity, making them a preferred choice for practical applications. When constructing them, we must also take into account the choice of pseudorandom number generators and the choice of low-discrepancy sequences. The described results are published in [36, 37].

2. Stochastic Resolvent Method: Development and Investigation of Efficient Algorithms for Minimum Eigenvalue

2.1 Problem Formulation

Let $A = \{a_{ij}\}_{i,j=1}^{n} \in \mathbb{R}^{n\times n}$ be a nonsingular symmetric matrix. The eigenvalues of A are defined as all real values of the parameter $\lambda(A)$ for which the equation

$$A\mathbf{x} = \lambda(A)\mathbf{x}, \qquad \text{where } \mathbf{x} \in \mathbb{R}^n, \tag{2.1}$$

has a nonzero solution. It is assumed that the eigenvalues satisfy the ordering

$$0 < \lambda_{\min} = \lambda_n < \lambda_{n-1} \leq \lambda_{n-2} \leq \cdots \leq \lambda_2 < \lambda_1 = \lambda_{\max}. \tag{2.2}$$

The minimal eigenvalue $\lambda_{\min}$ is positive and, according to (2.2), is unique. Consider the task of developing and investigating numerically efficient stochastic algorithms for its estimation.

2.2 Method for Computing Eigenvalues

Let $R = \{r_{ij}\}_{i,j=1}^{n} \in \mathbb{R}^{n\times n}$ be a nonsingular symmetric matrix whose eigenvalues satisfy the ordering:

$$\mu_{\min} = |\mu_n| < |\mu_{n-1}| \leq |\mu_{n-2}| \leq \cdots \leq |\mu_2| < |\mu_1| = \mu_{\max}, \tag{2.3}$$

and for which the equation:

$$R\mathbf{y} = \mu(R)\mathbf{y} \tag{2.4}$$

has a nonzero solution. From linear algebra theory, it is known that under certain relationships between the matrices R and A, there exist connections between their eigenvalues and eigenvectors. Three main cases are considered:

- For the inverse matrix $R = A^{-1}$, the eigenvalues are related by $\mu = \frac{1}{\lambda}$. This allows the use of the *Inverse Power* method to compute the minimal eigenvalue of A, but requires the expensive computation of the inverse matrix.
- For the shifted matrix $R_q = A - q\mathbf{I}$, the relation $\mu = \lambda - q$ holds. This leads to the *Shift Power* method, where the choice of the parameter q influences the approximation of the minimal eigenvalue.
- For the resolvent matrix $R_q = (\mathbf{I} - qA)^{-1}$, the eigenvalues are related by $\mu = \frac{1}{1-q\lambda}$, and the corresponding method is called the *Resolvent Power* method. The matrix R_q can be represented as the limit of an infinite convergent series under the condition $|q\lambda| < 1$, or equivalently $|q|\|A\| < 1$, namely:

$$R_q = \sum_{i=0}^{\infty} q^i A^i = [\mathbf{I} - qA]^{-1}. \tag{2.5}$$

Depending on the sign of the parameter q, different relations for the maximal eigenvalue are obtained:

$$\mu_{\max} = \frac{1}{1 - q\lambda_{\min}}, \qquad \text{for } q < 0, \tag{2.6}$$

$$\mu_{\max} = \frac{1}{1 - q\lambda_{\max}}, \qquad \text{for } q > 0. \tag{2.7}$$

Within the scope of the present study, the main interest is in the case $q < 0$, which enables accelerated approximation and efficient estimation of the extreme eigenvalues.

2.2.1 Resolvent Power Method

In the *classical* Power method, the largest eigenvalue $\lambda_{\max}$ of a symmetric matrix A is represented as the limit of the Rayleigh quotient (1.4), which allows a practical approximation using finite powers. On this basis, the Resolvent Power method is introduced, in which the resolvent matrix replaces the matrix A, $R_q = (\mathbf{I} - qA)^{-1}$,

which exists under the condition $|q|\|A\| < 1$. The resolvent matrix admits a Neumann series expansion, and its power R_q^m can be represented by a generalized binomial series:

$$R_q^m = (\mathbf{I} - qA)^{-m} = \sum_{i=0}^{\infty} q^i C_{i+m-1}^i A^i, \qquad C_{i+m-1}^i = \frac{(m+i-1)!}{(m-1)!i!}, \quad i = 0, 1, 2, \ldots. \tag{2.8}$$

The infinite series for R_q^m (where q is called the acceleration parameter) can be written as

$$R_q^m = (I - qA)^{-m} = \mathbf{I} + mqA + \frac{m(m+1)}{2} q^2 A^2 + \frac{m(m+1)(m+2)}{6} q^3 A^3 + \ldots. \tag{2.9}$$

Applying the Power method to the resolvent matrix (R_q) leads to the Resolvent Power method:

$$\lim_{m\to\infty} \frac{(\boldsymbol{h},\, R_q^m \boldsymbol{f})}{(\boldsymbol{h},\, R_q^{m-1} \boldsymbol{f})} = \lim_{m\to\infty} \frac{(\boldsymbol{h},\, (\mathbf{I} - qA)^{-m} \boldsymbol{f})}{(\boldsymbol{h},\, (\mathbf{I} - qA)^{-(m-1)} \boldsymbol{f})} = \mu_{\max} = \frac{1}{1 - q\lambda}, \tag{2.10}$$

which enables the computation of the maximal eigenvalue $\mu_{\max}$ of the resolvent matrix and, consequently, the estimation of the extreme eigenvalues of A. Depending on the sign of the parameter q, the method can be used to approximate $\lambda_{\max}$ or $\lambda_{\min}$, according to [19, 20, 22]:

$$\lambda = \frac{(\boldsymbol{h}, AR_q^m \boldsymbol{f})}{(\boldsymbol{h}, R_q^m \boldsymbol{f})} \approx \lambda_{\max}, \qquad \text{if } q > 0, \tag{2.11}$$

$$\frac{(\boldsymbol{h}, AR_q^m \boldsymbol{f})}{(\boldsymbol{h}, R_q^m \boldsymbol{f})} \approx \frac{1}{q}\left(1 - \frac{1}{\mu^{(m)}}\right) \approx \lambda_{\min}, \qquad \text{if } q < 0. \tag{2.12}$$

In practice, the resolvent matrix is approximated by truncating the series to a finite number of terms k:

$$R_{q,k}^m = \sum_{i=0}^{k} C_{i+m-1}^i q^i A^i, \tag{2.13}$$

which leads to a systematic error equal to the "tail" of the series:

$$\Delta_k^{(m)}(q) = (I - qA)^{-m} - R_{q,k}^m = \sum_{i=k+1}^{\infty} C_{i+m-1}^i q^i A^i. \tag{2.14}$$

Estimates for this error and conditions for selecting the parameters m and k such that it is smaller than a prescribed ε have been obtained, i.e.,

$$|\Delta_k^{(m)}(q)| < \varepsilon. \tag{2.15}$$

The following bound holds:

$$|\Delta_k^{(m)}(t)| \le T_{m,k}(t) = \sum_{i=k+1}^{\infty} C_{i+m-1}^i t^i, \qquad t = |q|\,|\lambda_{\max}| < 1. \tag{2.16}$$

There is a linear relationship between the parameters m and k under the condition $t = |q||\lambda_{max}| < 1$. The following estimates are obtained for the relationship between k and m:

- Accuracy inequality:

$$T_{m,k}(t) \le \frac{b_{k+1}}{1-\alpha} = \frac{\binom{m+k}{k+1} t^{k+1}}{1 - \frac{m+k+1}{k+2} t} < \varepsilon, \quad b_i = C_{i+m-1}^i t^i, \quad \alpha := \frac{m+k+1}{k+2}, \quad t < 1. \tag{2.17}$$

- Linear relations between the parameters:

$$m < \frac{1-t}{t}(k+1) + \frac{1}{t}, \qquad \text{or} \qquad m_{\max} = \left\lfloor \frac{(1-t)k+2}{t} - 1 \right\rfloor. \tag{2.18}$$

- Asymptotic relationship (for growing m and fixed t):

$$k \gtrapprox \frac{t}{1-t} m, \qquad \text{for large values of } m. \tag{2.19}$$

- Minimal value of k for fixed t:

$$k_{\min} = \left\lceil \frac{tm-1}{1-t} - 1 \right\rceil. \tag{2.20}$$

The derived relations enable an efficient choice of parameters in numerical implementations and form the basis for the construction of a Stochastic Resolvent method, including a balance between systematic and stochastic errors.

2.2.2 Stochastic Resolvent Method

The Stochastic Resolvent method, introduced by Karaivanova and Dimov [20, 25], represents a generalization of the Resolvent Power method to estimate the extreme eigenvalues of a matrix A. A fundamental component is the construction of random variables $\theta^{(i)}$, defined by a Markov chain, whose mathematical expectations coincide with the scalar products $(\boldsymbol{h}, A^i\boldsymbol{f}),\ i = 1, 2, 3, \ldots$, i.e.

$$E\big[\theta^{(i)}\big] = (\boldsymbol{h}, A^i\boldsymbol{f}), \qquad i = 1, 2, 3, \ldots. \tag{2.21}$$

Under the condition on the parameter q satisfying $|q\,\lambda_{max}| < 1$, it has been proven in [17] that the scalar product with the resolvent matrix can be represented as an infinite series:

$$(\boldsymbol{h},\, R_q^m\boldsymbol{f}) = (\boldsymbol{h},\, (\mathbf{I} - qA)^{-m}\boldsymbol{f}) = \sum_{i=0}^{\infty} q^i C_{i+m-1}^i E[\theta^{(i)}], \tag{2.22}$$

which allows for stochastic estimation using Monte Carlo methods. In practice, mathematical expectations are approximated by mean values:

$$\overline{\theta}_N^{(i)} = \frac{1}{N}\sum_{s=1}^{N}(\theta^{(i)})_s, \qquad i = 1, 2, 3, \ldots. \tag{2.23}$$

where the stochastic error is of the order of $\mathcal{O}(N^{-1/2})$. For a fixed accuracy ε, the problem of determining the minimum number of realizations N required to guarantee an error below a prescribed threshold has been solved under the assumptions of bounded variance and $||A|| < 1$:

$$N \geq \big\{\frac{c_k\,\sigma}{\varepsilon}\big\}^2. \tag{2.24}$$

Due to the truncation of the infinite series to a finite number of terms k, two errors arise: (1) stochastic (Monte Carlo approximation) and (2) systematic (from truncation of the series). The choice of parameters m and k controls the systematic error, and N controls the stochastic error. The balance between them is crucial for accuracy and computational efficiency. The approximate eigenvalue formula is as follows:

$$\lambda \approx \frac{E[\theta^{(1)}] + qC_m^1 E[\theta^{(2)}] + q^2 C_{m+1}^2 E[\theta^{(3)}] + \ldots + q^k C_{k+m-1}^k E[\theta^{(k+1)}]}{1 + qC_m^1 E[\theta^{(1)}] + q^2 C_{m+1}^2 E[\theta^{(2)}] + \ldots + q^k C_{k+m-1}^k E[\theta^{(k)}]}, \tag{2.25}$$

where the sign of the parameter q determines whether the maximum (λ_{max} at $q > 0$) or the minimum eigenvalue (λ_{min} at $q < 0$) is evaluated. When pseudorandom numbers are used, the method becomes the Resolvent Monte Carlo (RMC) method, whereas when low-discrepancy sequences are employed, it becomes the Resolvent Quasi-Monte Carlo (RQMC) method. The construction of random variables is based on an appropriate choice of the initial density and the transition probability matrix, and numerical results demonstrate a higher accuracy than *classical* deterministic algorithms.

2.3 Almost Optimal RMC and RQMC Methods and Algorithms

Let the matrix A be represented by the rows $\boldsymbol{a}_i$, introducing L_1-norms for vectors and matrices, which serve as a basis for constructing *almost optimal* stochastic resolvent algorithms. The choice of the initial density vector and the transition probability matrix is implemented by normalizing the absolute values of the components of $\boldsymbol{h}$ and the rows of matrix A, which leads to an *almost optimal* structure of the Markov chain.
The *almost optimal* Resolvent Quasi-Monte Carlo (RQMC) algorithm is presented for estimating the minimal eigenvalue of a symmetric matrix. The algorithm employs low-discrepancy sequences (for example, a scrambled Sobol sequence) to generate realizations in the Markov chain and to compute the random variables $\theta^{(i)}$. When pseudorandom generators are used, the method reduces to an *almost optimal* Resolvent Monte Carlo (RMC)

algorithm. In Step 4 of the algorithm, a scrambled Sobol sequence is used as a low-discrepancy sequence to compute the values of the random variables $\theta^{(i)},\ i = 1, 2, \ldots, k+1$, via a Markov chain.
Algorithm 2 is presented in pseudocode and describes the *almost optimal* RQMC algorithm to estimate the minimal eigenvalue of the symmetric matrix A. If pseudorandom number generators (PRNGs) are used in Step 4, the algorithm is referred to as the *almost optimal* RMC algorithm. In the following exposition, the *almost optimal* RMC algorithm will be denoted by **Algorithm 2a**. Both algorithms belong to the class of iterative stochastic methods and are characterized by the presence of two types of errors: stochastic and systematic. The stochastic error in the MC methods is of the order of $\mathcal{O}(N^{-1/2})$, while in the QMC methods based on low-discrepancy sequences it is $\mathcal{O}(N^{-1}(logN)^k)$. High dimensionality may lead to correlations between the coordinates of quasirandom sequences, which can be mitigated by using scrambled quasirandom sequences.

Algorithm 2 Pseudocode for computing the *almost optimal* Resolvent QMC algorithm

1: INPUT: matrix $A = \{a_{ij}\} \in \mathbb{R}^{n\times n}$; vectors $\boldsymbol{h}, \boldsymbol{f} \in \mathbb{R}^n$, positive integers n, N, k, m and the real number q, where $(-1)/\|A\| < q < 0$

2: COMPUTE: $p_i = \frac{|h_i|}{\sum_{i=1}^n |h_i|}; p_{ij} = \frac{|a_{ij}|}{\sum_{j=1}^n |a_{ij}|},\ 1 \le i \le n,\ 1 \le j \le n$

3: COMPUTE: $a_i = \sum_{j=1}^n |a_{ij}|,\ \ 1 \le i \le n,\ \ \|\boldsymbol{h}\| = \sum_{i=1}^n |h_i|$

4: GENERATE: N elements of the $(k+1)$ - dimensional Sobol sequence

5: CONSTRUCT: N realizations of the Markov chain with integer elements

$$l_1^{(s)} \to \ldots \to l_i^{(s)} \to \cdots \to l_k^{(s)} \to\ l_{k+1}^{(s)},\ 1 \le l_i^{(s)} \le n,\ 1 \le i \le k+1,\ 1 \le s \le N$$

6: COMPUTE:

$$\overline{\theta}^{(i)} = \frac{1}{N} \parallel \boldsymbol{h} \parallel \sum_{s=1}^{N} sign\{h_{l_1^{(s)}} \prod_{i=1}^{k+1} (a_{l_i^{(s)} l_{i+1}^{(s)}})\} \prod_{i=1}^{k+1} a_{l_i^{(s)}} f_{l_{i+1}^{(s)}};\ \ 1 \le i \le k+1$$

7: COMPUTE:

$$C_{i+m-1}^i = \frac{(i+m-1)!}{i!(m-1)!}, \text{where}\ \ 1 \le i \le k$$

8: OUTPUT:

$$\lambda_{min} \approx \frac{\overline{\theta}^{(1)} + qC_m^1\overline{\theta}^{(2)} + q^2C_{m+1}^2\overline{\theta}^{(3)} + ... + q^kC_{k+m-1}^k\overline{\theta}^{(k+1)}}{1 + qC_m^1\overline{\theta}^{(1)} + q^2C_{m+1}^2\overline{\theta}^{(2)} + ... + q^kC_{k+m-1}^k\overline{\theta}^{(k)}}$$

The systematic error arises from the use of a finite (truncated) Markov chain and is analogous to the truncated Neumann series in deterministic methods. It depends on the truncation parameter k in the representation of the resolvent matrix $R_{q,k}^m$ as a limit of infinite order under the condition $|q|||A|| < 1$. The parameter m determines the degree of the resolvent matrix and affects the convergence of the method:

$$\mathcal{O}\left(|\frac{\mu_2}{\mu_1}|^m\right), \tag{2.26}$$

where μ_1, μ_2 are the largest eigenvalues of the resolvent matrix. Expressed in terms of the eigenvalues of A :

$$\mathcal{O}\left(\left|\frac{1-q\lambda_1}{1-q\lambda_2}\right|^m\right),\ \text{for}\ \ q > 1 \text{ and } \mathcal{O}\left(\left|\frac{1-q\lambda_n}{1-q\lambda_{n-1}}\right|^m\right),\ \text{for}\ \ q < 1. \tag{2.27}$$

The choice of the acceleration parameter q determines whether the algorithm evaluates the minimum ($q \in (-\frac{1}{||A||}, 0)$) or the maximum eigenvalue ($q > 0$). The computational process involves generating N realizations of the Markov chain, computing sample means for the random variables, and using binomial coefficients to estimate the eigenvalue.
The balance between stochastic and systematic error is essential for achieving a prescribed accuracy ε at optimal computational cost. This balance is controlled through the parameters N (number of realizations), k (chain length), m (resolvent power), and q (acceleration parameter). Numerical experiments demonstrate that the choice of these parameters must be consistent with the derived theoretical convergence estimates.

2.4 Numerical Results and Discussion

The numerical results were obtained by applying the *almost optimal* Resolvent Quasi-Monte Carlo (RQMC) algorithm (**Algorithm 2**) and the *almost optimal* Resolvent Monte Carlo (RMC) algorithm (**Algorithm 2a**) to estimate the minimal eigenvalue of randomly generated symmetric matrices of sizes $n = 500$ and $n = 1000$. The *almost optimal* RQMC algorithm is implemented using BRODA's Sobol RSG generator, which enables the generation of scrambled Sobol sequences with the required dimensionality for constructing the Markov chain. The *almost optimal* RMC algorithm is implemented using the Mersenne Twister (MT) pseudorandom number generator. Both algorithms are implemented in C++, with a preliminary subroutine used to generate a random symmetric matrix A whose spectrum lies within the unit circle and satisfies the following condition:

$$0 < c < \lambda_n < \lambda_{n-1} \leq \ldots \leq \lambda_2 < \lambda_1 < 1,$$

where the constant $\boldsymbol{c}$ is chosen to be $c = 0.15$. This guarantees positivity and spectral separation, which are necessary for the convergence of the resolvent power method.
Two test cases are considered:

(i) Matrix A of dimension $n = 500$, with the two largest and two smallest eigenvalues being: $\lambda_1 = 0.620713$, $\lambda_2 = 0.335683$, $\lambda_{499} = 0.15452$ and $\lambda_{500} = 0.152992$.

(ii) Matrix A with dimension $n = 1000$, with the two largest and two smallest eigenvalues being: $\lambda_1 = 0.688181$,$\lambda_2 = 0.443078$, $\lambda_{999} = 0.154138$ and $\lambda_{1000} = 0.151911$.

The separation between the two largest and the two smallest eigenvalues ensures a reliable convergence of the method when estimating λ_{min}.
The numerical experiments are conducted on a high-performance computing cluster (IICT–BAS), consisting of 12 Fujitsu Primergy RX 2540 M4 servers, each configured with: 128 GB RAM; two CPUs – Intel Xeon Gold 5118 (2.30 GHz) with 24 cores; two 800 GB SSDs; 36 TB HDD; and an NVIDIA Tesla V100 GPU with 32 GB memory. The servers are interconnected via InfiniBand for fast, low-latency data exchange. The installed software includes Red Hat Enterprise Linux 7.6 and NVIDIA GRID.
The implementation of **Algorithm 2** is hybrid: the generation of scrambled Sobol sequences is performed on the GPU (NVIDIA Tesla V100, 5120 CUDA cores), while the remaining computations are executed on the CPU. **Algorithm 2a** is implemented on the CPU using the Mersenne Twister generator.
The arbitrarily vectors $\boldsymbol{h}$ and $\boldsymbol{f}$ are chosen with a L_1-norm as follows:

$$\|\boldsymbol{h}\| = \|\boldsymbol{f}\| = \sum_{i=1}^{n} \frac{1}{n} = 1,$$

to ensure proper normalization in the stochastic estimations. Numerical tests show that for large values of the number of realizations N, the execution time of the RQMC algorithm ($RQMC_{(S)}$) is significantly lower than that of the RMC algorithm ($RMC_{(MT)}$). They demonstrate the advantage of the Quasi-Monte Carlo approach combined with GPU acceleration in large-scale problems for estimating the minimal eigenvalue.

2.4.1 Case (i): Matrix size *n=500*

Table 2.1 presents numerical results to estimating the minimum eigenvalue of a symmetric matrix of dimension $n = 500$, obtained by the *almost optimal* algorithms ($RMC_{(MT)}$ and $RQMC_{(S)}$) for different values of the parameters N, k and m. The table also includes the corresponding absolute errors of the estimates obtained. The acceleration parameter is fixed at $q = -0.157428$, and the systematic error is preset at the level $\varepsilon_{sys} = 0.001$.
The analysis of the results is based on the balancing of the two main sources of error - systematic and stochastic. The systematic error arises from the truncation of the Neumann series at $i = k + 1$, which corresponds to a finite number of transitions in the Markov chain, as well as from the choice of the degree m of the resolvent matrix. The parameters m and k are chosen based on theoretical estimates of the tail of the series $T_{m,k}(t)$, for $t = |q||\lambda_1| < 1$, so that the condition $T_{m,k}(t) \leq \varepsilon_{sys} = 0.001$ is satisfied. In this way, the systematic error is controlled in advance and remains on the order of $\mathcal{O}(10^{-3})$.
The stochastic error arises from the approximation of mathematical expectations by a finite number of realizations N. In the Monte Carlo approach ($RMC_{(MT)}$), the stochastic error is on the order of $\mathcal{O}(N^{-1/2})$ for a fixed confidence probability. In the Quasi-Monte Carlo approach ($RQMC_{(S)}$), faster convergence is expected. To estimate the statistical error, scrambled Sobol sequences are used, which combine low-discrepancy properties with controlled randomness. It should be noted that the stochastic error depends not only on N, but also on the parameter k; increasing k increases the number of estimated random variables $\theta^{(i)}$, $i = 1, \ldots, k + 1$.

Table 2.1: Numerical results for the matrix $A \in \mathbb{R}^{500\times500}$ for different values of N, k and m with the acceleration parameter $q = -0.157428$. The exact minimum eigenvalue $\lambda_{\min} = \lambda_{500} = 0.152992$.

N	k	m	λ_{min} $RMC_{(MT)}$	Absolute error $RMC_{(MT)}$	λ_{min} $RQMC_{(S)}$	Absolute error $RQMC_{(S)}$
$512 * 2^0$	5	5	0.1585637	0.0055717	0.1561046	0.0031126
	5	10	0.1585163	0.0055243	0.1524884	**0.0005036**
	10	5	0.1556132	**0.0026212**	0.1560595	0.0030675
$512 * 2^1$	5	5	0.158395	0.005403	0.1596503	0.0066583
	5	10	0.1585518	0.0055598	0.1595946	0.0066026
	10	5	0.1580794	0.0050874	0.1596616	0.0066696
$512 * 2^5$	5	5	0.1572588	0.0042668	0.1591139	0.0061219
	5	10	0.1566524	0.0036604	0.1585388	0.0055468
	10	5	0.156875	0.003883	0.1591292	0.0061372
$512 * 2^6$	5	5	0.157129	0.004137	0.1589384	0.0059464
	5	10	0.1565796	0.0035876	0.1584563	0.0054643
	10	5	0.1570216	0.0040296	0.158961	0.005969

This leads to the accumulation of variances in both the numerator and the denominator of the rational formula for estimating eigenvalues, which affects the required number of realizations. Therefore, an effective balance requires selecting N so that the stochastic error is of the same order as the prescribed systematic error ε_{sys}.

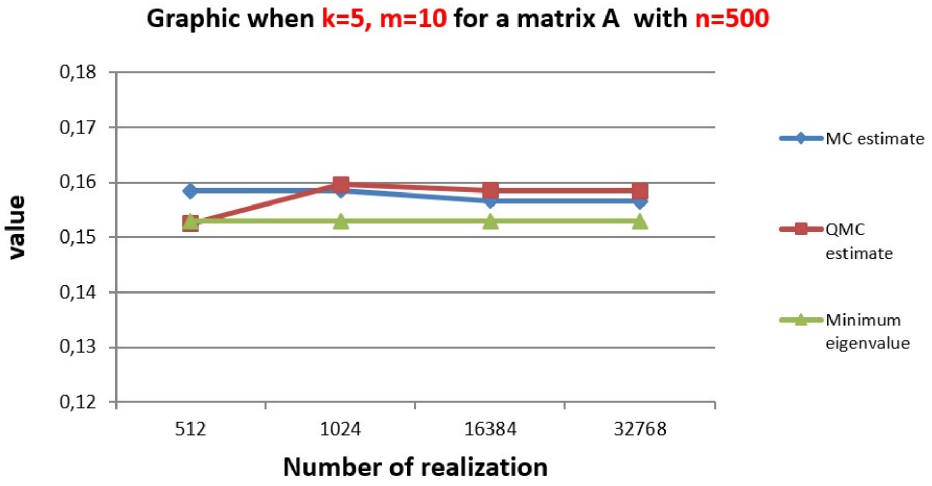


Figure 2.1: Convergence to the exact minimum eigenvalue of the matrix A using MC and QMC at $k = 5, m = 10$ for different values of N

The results obtained for $n = 500$ confirm the theoretical conclusions. With an appropriate choice of parameters (m, k), which guarantee a limitation of the systematic error below $\mathcal{O}(10^{-3})$, high precision is achieved even with a relatively small number of realizations N, comparable to the dimensionality of the matrix. The best accuracy is obtained at $k = 5$, $m = 10$, and $N = 512$, where the absolute error is of the same order as the previously specified systematic error. Increasing N (for example, to $N = 16384$ or $N = 32768$, see Figure 2.1 and Table 2.1) does not lead to a monotonic decrease in absolute error.
Saturation or oscillating behavior is observed, which is characteristic of situations in which the systematic error already determines the lower limit of accuracy. Additional influence is exerted by numerical effects associated with the increase in binomial coefficients at larger values of m and k, which increase the sensitivity of the fractional-rational formula to small fluctuations in estimates of $\theta^{(i)}$. Therefore, increasing N does not automatically guarantee improved accuracy when the systematic component or the numerical sensitivity of the method becomes dominant.

2.4.2 Case (ii): Matrix size *n=1000*

Table 2.2 presents numerical results for estimating the minimum eigenvalue of a symmetric matrix of dimension $n = 1000$, obtained by the *almost optimal* algorithms $RMC_{(MT)}$ and $RQMC_{(S)}$, together with the corresponding absolute errors. In these experiments, the acceleration parameter is fixed at $q = -0.2302458$, and its absolute value is higher compared to the case $n = 500$. This increases the parameter $t = |q||\lambda_1|$ and requires, for the same values of k and m, that the systematic error be fixed at a higher level $\varepsilon_{sys} = 0.01$ to satisfy the theoretical conditions to estimate the tail of the series.

Table 2.2: Numerical results for the matrix $A \in \mathbb{R}^{1000\times1000}$ for different values of N, k and m with acceleration parameter $q = -0.230245$. The exact minimum eigenvalue $\lambda_{\min} = \lambda_{1000} = 0.151911$.

N	k	m	λ_{min} $RMC_{(MT)}$	Absolute error $RMC_{(MT)}$	λ_{min} $RQMC_{(S)}$	Absolute error $RQMC_{(S)}$
$512 * 2^0$	5	5	0.1556059	0.0045949	0.1705751	0.0186641
	5	10	0.168251	0.01634	0.1886959	0.0367849
	10	5	0.1593428	0.0074318	0.1701307	0.0182197
$512 * 2^1$	5	5	0.1504153	**0.0014957**	0.1533797	**0.0014687**
	5	10	0.1417805	0.0101305	0.1499974	0.0019136
	10	5	0.156739	0.004828	0.1534383	0.0015273
$512 * 2^5$	5	5	0.1550015	0.0030905	0.1573842	0.0054732
	5	10	0.1495483	0.0023627	0.1539357	0.0020247
	10	5	0.1559548	0.0040438	0.1575454	0.0056344
$512 * 2^6$	5	5	0.1557509	0.0038399	0.1576339	0.0057229
	5	10	0.1537008	0.0017898	0.1562911	0.0043801
	10	5	0.1562905	0.0043795	0.15764225	0.0057312

The results (see Table 2.2 and Figure 2.2) show that the best balance between the systematic and stochastic components of the error is achieved at $k = 5$, $m = 5$, and $N = 1024$. For this combination, the absolute error is minimal and of the same order as the prescribed systematic error. This confirms the theoretical conclusion that the parameters m and k, determined based on a fixed level of systematic error, ensure the required accuracy of the approximation of the resolvent matrix, while the number of realizations N should be chosen so that the stochastic error is comparable to the systematic one. For higher values of m, k and N, a certain improvement of the absolute error is observed in terms of the constant factor, but without a change in order, while the computational complexity increases. Increasing N (for example, to $N = 16384$ or $N = 32768$, see Figure 2.2 and Table 2.2) does not lead to a monotonic decrease in the error. The reason is due to the increased sensitivity of the rational formula to small fluctuations in the estimates of the random variables $\theta^{(i)}$, as well as the dominant role of the systematic error.

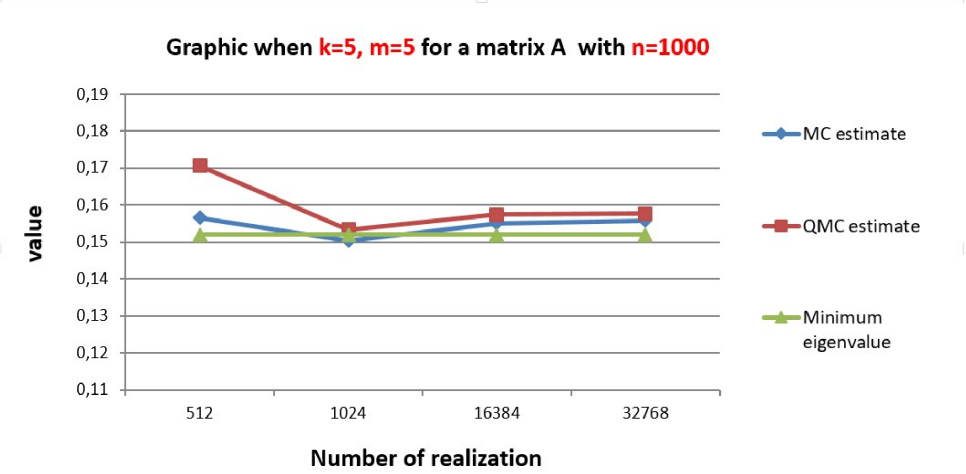


Figure 2.2: Convergence to the exact minimum eigenvalue of the matrix A using MC and QMC at $k = 5, m = 5$ for different values N

In practice, the results indicate that for matrices of dimension on the order of several thousand, an optimal balance is achieved when m and k are chosen according to theoretical estimates at a pre-fixed level of systematic

error, and N is of the same order as the matrix dimension. Too small N leads to a dominant stochastic error, while too large N increases the computational cost without a significant improvement in accuracy.

2.5 Summary

Estimating the minimum eigenvalue λ_{min} of a symmetric matrix using stochastic power algorithms requires the computation of the inverse matrix A^{-1}, which is computationally expensive for large dimensions. As an efficient alternative, the Stochastic Resolvent method is investigated, which eliminates the need to explicitly calculate A^{-1} by using the resolvent matrix $R_q = (\mathbf{I} - qA)^{-1}$ and its powers. The sign of the acceleration parameter q determines whether the minimum or maximum eigenvalue is estimated.
Theoretical analysis shows that the convergence of the Resolvent Power method is essentially dependent on the parameter q and the power m. The systematic error decreases as m increases, while the ratio of the extreme eigenvalues of the matrix determines the convergence rate. The truncation of the binomial series through the parameter k introduces an additional systematic error, from which analytical estimates are derived. A linear dependence between m and k is established, enabling the selection of minimal values at a fixed level of systematic error and thereby reducing computational complexity.
In stochastic implementation, a stochastic error also arises. *Almost optimal* RMC and *almost optimal* RQMC algorithms are proposed, in which mathematical expectations are approximated by sample averages of N realizations of a truncated Markov chain with k transitions. In the MC approach, the error is of order $\mathcal{O}(N^{-1/2})$. In contrast, QMC methods use the Koksma-Hlawka inequality together with low-discrepancy sequences (e.g., Sobol sequences), providing faster convergence. The general accuracy is determined by the balance between systematic error (due to truncation of the series) and stochastic error (due to the finite number of realizations), which requires a balanced choice of the parameters m, k, and N.
The theoretical estimates obtained provide practical guidelines for selecting m, k, and N so that both types of errors are of comparable order with respect to the prescribed accuracy. Numerical experiments for matrices of dimensions $n = 500$ and $n = 1000$ confirm these conclusions: the best efficiency is achieved for parameter choices corresponding to the theoretically predicted balance, and increasing N beyond a certain threshold does not lead to significant improvement. The *almost optimal* RQMC algorithm demonstrates faster convergence compared to the MC approach, and the hybrid GPU/CPU implementation enables efficient application to high-dimensional problems. Part of the results presented in this chapter are published in the articles [35, 36].

3. Stochastic methods for assessing the market risk of investment portfolios

This chapter presents an application of **Algorithm 1** to a real-world problem in financial mathematics: assessing market risk in an investment portfolio. The aim is to demonstrate the practical applicability of stochastic power algorithms by analyzing the spectral characteristics of the correlation matrix of asset returns. Estimating extreme eigenvalues enables the identification of dominant risk factors and the examination of the portfolio's sensitivity to market fluctuations. In this way, theoretical algorithms are employed as tools for quantitative risk analysis and to support investment decision-making.

3.1 Problem Formulation

The main task addressed in this chapter is to estimate the maximum eigenvalue of correlation matrices and to analyze the accuracy of the estimates obtained by applying *almost optimal* Power Monte Carlo (PMC) and *almost optimal* Power Quasi-Monte Carlo (PQMC) algorithms, presented in Chapter 1. These algorithms are used to estimate the largest eigenvalue of the matrices numerically and to investigate the approximation error. Within the PQMC algorithm, two additional operators are introduced: (1) a skipping operator and (2) a leaping operator. Their use is motivated by the need to reduce the influence of initial irregularities inherent in randomized low-discrepancy sequences.

3.2 Methods and Data

The financial data used to construct the correlation matrices are extracted from the *Portfolio Visualizer* and *Yahoo Finance* platforms, with access to the latter provided through the *yFinance* library. The estimation of the largest eigenvalue of the correlation matrices is performed using the algorithms specified in Chapter 1 and the balance between systematic and stochastic error is analyzed. For interpretation of the results in the context of financial analysis, the *Fraction of Variance Explained* (FVE) indicator is used, which measures the share of the explained variation corresponding to the maximum eigenvalue and characterizes the degree of influence of the dominant market factor.

3.3 General Formulation of Covariance and Correlation Matrices

Covariance and the correlation coefficient are fundamental characteristics for describing the linear dependence between random variables. The covariance between two random variables X and Y is defined as

$$Cov(X,Y) = E\left[(X-\mu_X)(Y-\mu_Y)\right], \tag{3.1}$$

where $\mu_X = E[X]$ and $\mu_Y = E[Y]$ [77, 91]. It measures the direction of joint variability and can take both positive and negative values, but it depends on the scale of the variables.
The correlation coefficient represents a normalized form of covariance and is given by:

$$Corr(X,Y) = \rho_{XY} = \frac{Cov(X,Y)}{\sigma_X \sigma_Y}, \tag{3.2}$$

where σ_X and σ_Y are the standard deviations [77, 91]. It takes values in the interval $[-1,1]$ and allows for the comparison of linear dependencies independently of the measurement units.
For a random vector $\mathbf{X} = (X_1, \ldots, X_n)^T$, the covariance matrix is defined as

$$\Sigma = Cov(\mathbf{X}) = E\left[(\mathbf{X}-\mu)(\mathbf{X}-\mu)^T\right], \tag{3.3}$$

where the elements $\Sigma_{ij} = Cov(X_i, X_j)$ and the diagonal elements $\Sigma_{ii} = \sigma_i^2$ represent the variances. Accordingly, the correlation matrix is defined as:

$$\hat{R} = [\rho_{ij}]_{i,j=1}^n, \quad \rho_{ij} = Corr(X_i, X_j), \quad i,j = 1,\ldots,n, \tag{3.4}$$

with $\rho_{ii} = 1$ [42, 57].

In the context of portfolio analysis, the correlation matrix describes the relationships between asset returns, while its largest eigenvalue indicates the dominant market factor [42]. High values of this characteristic are associated with increased market synchronization and limited diversification opportunities. The covariance matrix, in turn, provides complete information about the interdependencies between assets and is a fundamental tool in portfolio optimization and risk management.

3.3.1 Construction of Covariance and Correlation Matrices from Empirical Financial Data

In empirical studies of financial markets, data are typically represented as a matrix $B \in \mathbb{R}^{r\times n}$, where the rows correspond to time points and the columns correspond to the returns of different assets. Each row $\mathbf{b}_i$ describes the joint market state at a given time, allowing analysis of interdependencies between assets. The matrix B is defined as

$$B = [b_{ij}]_{i,j=1}^{r,n} = (\mathbf{b}_1, \ldots, \mathbf{b}_i, \ldots, \mathbf{b}_r)^T, \tag{3.5}$$

where each row $\mathbf{b}_i$ represents a vector of observed returns for all assets at time i. This representation forms the basis for statistical analysis and the construction of covariance and correlation structures.

Data Centering and Sample Covariance and Correlation Matrices

Let $\overline{\mathbf{b}}$ be the n-dimensional vector of sample column means of matrix B. The centered matrix is defined as follows:

$$B_c = B - \mathbf{e}\overline{\mathbf{b}}^T, \tag{3.6}$$

where $\mathbf{e} \in \mathbb{R}^r$ is a vector of units. The sample covariance matrix is defined as:

$$\Sigma = \frac{1}{r} B_c^T B_c. \tag{3.7}$$

For small values of r in formula (3.7), the division is performed by $r-1$. The elements Σ_{ij} measure the joint variability between asset returns, and the diagonal elements Σ_{ii} correspond to their variations. The risk of a portfolio Π with weights $\mathbf{w}$ is given by the quadratic form:

$$Var(\Pi) = \mathbf{w}^T \Sigma \mathbf{w}, \tag{3.8}$$

which emphasizes the role of both individual risks and interdependencies between assets. The correlation matrix is obtained by normalizing the covariance matrix with the standard deviations:

$$\hat{R} = D_\sigma^{-1/2} \Sigma D_\sigma^{-1/2}, \qquad \rho_{ij} = \frac{\Sigma_{ij}}{\sigma_i \sigma_j}, \tag{3.9}$$

where $\rho_{ij} \in [-1, 1]$ and $\rho_{ii} = 1$. This matrix provides a scale-independent measure of linear relationships between assets and is key to the analysis of diversification [42].

3.3.2 Fraction of Variance Explained

The Fraction of Variance Explained (FVE) is an important characteristic related to the spectral properties of covariance or correlation matrices [47]. Let A be a symmetric matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$. Then FVE for the largest eigenvalue is defined as:

$$FVE_1 = \frac{\lambda_1}{\sum_{j=1}^n \lambda_j} = \frac{\lambda_1}{trace(A)}, \tag{3.10}$$

and for the first k components:

$$FVE_k = \frac{\sum_{i=1}^k \lambda_i}{trace(A)}. \tag{3.11}$$

In the special case of a correlation matrix $\hat{R}$, for which $trace(\hat{R}) = n$, we obtain:

$$FVE_1 = \frac{\lambda_1}{n}. \tag{3.12}$$

This quantity measures the relative contribution of the dominant factor to the total variance of the system. In

the context of financial markets, high values of FVE_1 indicate the presence of a strong common market factor and a high level of systematic risk, which limits the efficiency of diversification. In contrast, lower values suggest a more balanced distribution of risk between independent factors and more favorable conditions for portfolio optimization. Therefore, estimating the largest eigenvalue of the correlation matrix and the corresponding fraction of variance explained is a key step in quantitative market risk analysis.

3.3.3 Stochastic Algorithms for Estimation of the Maximum Eigenvalue of a Correlation Matrix

When estimating the largest eigenvalue of the considered correlation matrices, the *almost optimal* Power Monte Carlo (PMC) and Power Quasi-Monte Carlo (PQMC) algorithms developed in Chapter 1 are applied. These algorithms demonstrate significant superiority over their *classical* counterparts, providing higher numerical accuracy and more stable convergence of estimates at comparable computational costs.
The *almost optimal* PQMC algorithm (**Algorithm 1**) uses low-discrepancy scrambled sequences to construct a Markov chain over a finite number of steps. In particular, in Step 4, Halton and Sobol sequences are generated using the corresponding pseudocodes **Algorithm 3** and **Algorithm 4**.

Algorithm 3 Pseudocode for generating a scrambled Halton Sequence with *skip* and *leap* parameters

1: CREATE FUNCTION: `generateHaltonSequence` (N, k+1)
2: GENERATE: $p \leftarrow$ `haltonset`(k, `'skip'` = s_1, `'leap'` = l_1)
3: GENERATE: $p \leftarrow$ `scramble`(p, 'RR2')
4: GENERATE: *points* $\leftarrow$ `net`(p, N)
5: OUTPUT: Return *points*

Algorithm 4 Pseudocode for generating a scrambled Sobol Sequence with *skip* and *leap* parameters

1: CREATE FUNCTION: `generateSobolSequence` (N, k+1)
2: GENERATE: $p \leftarrow$ `sobolset`(k, `'skip'` = s_1, `'leap'` = l_1)
3: GENERATE: $p \leftarrow$ `scramble`(p, 'MatousekAffineOwen')
4: GENERATE: *points* $\leftarrow$ `net`(p, N)
5: OUTPUT: Return *points*

When $s_1 = 0$ and $l_1 = 0$ are chosen, standard (*default*) versions of the sequences are obtained, respectively denoted by $PQMC^{(d)}_{(H)}$ and $PQMC^{(d)}_{(S)}$. For non-zero values of the parameters, the operations *skip* and *leap* are applied, which allow control over the initial elements and the thinning of the sequences, and the corresponding algorithms are denoted by $PQMC^{(s,l)}_{(H)}$ and $PQMC^{(s,l)}_{(S)}$.
For the implementation of the *almost optimal* PMC algorithm (**Algorithm 1a**), the pseudorandom number generators *Mersenne Twister* (MT) and *Middle Square* (MS) are used, with the corresponding variants denoted by $PMC_{(MT)}$ and $PMC_{(MS)}$. All algorithms are implemented in the MATLAB environment (version 9.10, R2021a), and the syntax used for the `haltonset`, `sobolset`, and `scramble` functions in **Algorithm 3** and **Algorithm 4** is consistent with the official documentation of MATLAB [93, 94].

3.4 Numerical Results and Discussion

This section presents numerical results for estimating the maximum eigenvalue of two correlation matrices using the *almost optimal* PMC and PQMC algorithms. The study was conducted on two asset portfolios with different dimensions, which allows for analysis of the behavior of the algorithms at different levels of complexity and information saturation of the data.
The first correlation matrix is constructed from the monthly returns of $n = 32$ global assets for the period January 2007-March 2024, with dimensions $r = 207$ and $n = 32$. The second matrix is constructed from the returns of $n = 490$ companies in the $S\&P500$ index for the period 2021-2025, with $r = 5$. By applying centering (i.e., formula (3.6)), estimation of the covariance matrix (3.7) and normalization (3.9), correlation matrices with corresponding maximum eigenvalues and FVE are obtained:

- for $n = 32$: $\lambda_{max} = 18.14714$, $FVE_1 = 56.71\%$;
- for $n = 490$: $\lambda_{max} = 201.090512$, $FVE_1 = 41.04\%$.

These values are calculated using the built-in functions of MATLAB and serve as a reference for assessing the accuracy of the algorithms.
In the numerical experiments, the vectors $\boldsymbol{h}$ and $\boldsymbol{f}$, used in the construction of $\theta^{(k)}$ and $\theta^{(k-1)}$, are chosen with a L_1-norm:

$$\|\boldsymbol{h}\| = \|\boldsymbol{f}\| = \sum_{i=1}^{n} \frac{1}{n} = 1.$$

which provides normalization and stability of the stochastic estimates. To ensure convergence, the matrix $A = q\hat{R}$ is considered, with the parameter q chosen such that condition $||A|| < 1$ is satisfied:

$$q = \frac{1}{|\lambda_1| + \delta}, \qquad \delta > 0.$$

or in the absence of a prior estimate for λ_1:

$$q = \frac{1}{\|\hat{R}\|_1 + \delta}, \qquad \|\hat{R}\|_1 = \max_{1 \le j \le n} \sum_{i=1}^{n} |\rho_{ij}| \qquad \text{and} \qquad \delta > 0.$$

This approach ensures the correct applicability of stochastic methods and guarantees their numerical robustness in estimating the maximum eigenvalue.

3.4.1 Case (i): correlation matrix with dimension $n = 32$

Table 3.1 presents the numerical results for estimating the largest eigenvalue of the correlation matrix $\hat{R}$ with dimension $n = 32$. The numerical results obtained are implemented by the *almost optimal* PMC algorithm (**Algorithm 1a**), using two pseudorandom number generators: *Mersenne Twister* (MT) and *Middle Square* (MS), respectively, denoted by $PMC_{(MT)}$ and $PMC_{(MS)}$. The estimation of the maximum eigenvalue $\lambda_1 = \lambda_{\max}$ was performed for different values of the number of transitions k in the Markov chain and the number of realizations N of the random variables $\theta^{(k)}$ and $\theta^{(k-1)}$, and the corresponding absolute errors are presented in Table 3.1. The analysis shows that for a fixed N, increasing k leads to a decrease in error. It stabilizes around $k = 8$, indicating that a practically optimal balance has been reached between the systematic and stochastic components of the error. On the other hand, with an increase in N, a monotonic decrease in absolute error is observed, which is in accordance with the *classical* properties of Monte Carlo methods.
The minimum absolute errors for the two algorithms are noted in Table 3.1, and the results show a comparable order of accuracy for both generators. The visualization in Figure 3.1 illustrates the convergence of the estimates $\lambda_1^{(k)}$ to the exact value λ_1 for a fixed $k = 8$ and an increasing number of realizations N. It is observed that both algorithms tend to the reference value, but $PMC_{(MT)}$ demonstrates higher accuracy and more stable convergence, especially for smaller N. In practice, to achieve accuracy in the second or third decimal place, simulations of $N = 512$ or $N = 1024$ are sufficient, which is fully adequate for applications in portfolio analysis. Using formula (3.12) for a correlation matrix of dimension $n = 32$ and estimates at $N = 1024$, we obtain values $\text{FVE}_1 \approx 56.70\%$ for $PMC_{(MT)}$ and $\text{FVE}_1 \approx 56.72\%$ for $PMC_{(MS)}$. This confirms that approximations of λ_1 with precision on the order of $\mathcal{O}(10^{-3})$ enable a reliable calculation of the fraction of explained variation, a key indicator for assessing systematic risk and the collective dynamics of assets. Therefore, the *almost optimal* PMC algorithm is an effective tool for analyzing correlation structures of moderate dimension at relatively low computational costs.
Table 3.2 presents the results of the application of the *almost optimal* PQMC algorithm for the same correlation matrix ($n = 32$), implemented through four variants: $PQMC_{(H)}^{(d)}$, $PQMC_{(S)}^{(d)}$, $PQMC_{(H)}^{(s,l)}$, and $PQMC_{(S)}^{(s,l)}$. The variants with index (d) correspond to the choice of $s_1 = 0$ and $l_1 = 0$ in **Algorithm 3** and **Algorithm 4**, i.e., using scrambled Halton and Sobol sequences with default settings. For non-zero values of the parameters *skip* and *leap*, the (s, l) variants are implemented, which allow finer control over the uniformity of the generated points and potentially improve the convergence of the estimates.
The numerical results for the *almost optimal* PQMC algorithms $PQMC_{(H)}^{(s,l)}$ and $PQMC_{(S)}^{(s,l)}$ were obtained by choosing the parameters $s_1 = 1024$ and $l_1 = 128$ in **Algorithm 3** and **Algorithm 4**, which corresponds to applying the *skip* and *leap* operations when generating the scrambled Halton and Sobol sequences. The maximum eigenvalue $\lambda_1 = \lambda_{\max}$ of the correlation matrix was estimated for different values of the number of transitions k and the number of realizations N, and the corresponding absolute errors are presented in Table 3.2. The results show that the parameters k and N significantly affect the balance between systematic and stochastic errors, as well as the computational complexity of the algorithms. At a fixed N, increasing k leads to a decrease

Table 3.1: Results for the maximum values of $\lambda_{max}^{(k)}$ and the absolute error for $PMC_{(MT)}$ and $PMC_{(MS)}$ at different N and k when $\lambda_{max} = 18.14714$

N	k	$\lambda_1^{(k)}$ using $PMC_{(MT)}$	Absolute Error $PMC_{(MT)}$	$\lambda_1^{(k)}$ using $PMC_{(MS)}$	Absolute Error $PMC_{(MS)}$
128	5	17.809541	0.3376	17.766635	0.3805
	6	17.955782	0.1914	17.931153	0.2160
	7	18.031908	0.1152	18.016774	0.1304
	8	**18.178382**	**0.0312**	**18.184488**	**0.0373**
	9	18.217756	0.0706	18.234182	0.0870
	10	18.259830	0.1127	18.278015	0.1309
	11	18.293246	0.1461	18.336586	0.1894
256	5	17.886432	0.2607	17.880110	0.2670
	6	18.013889	0.1333	18.025125	0.1220
	7	18.098671	0.0485	18.090287	0.0569
	8	**18.163375**	**0.0162**	**18.172589**	**0.0254**
	9	18.214595	0.0675	18.220052	0.0729
	10	18.265757	0.1186	18.270934	0.1238
	11	18.307841	0.1607	18.317397	0.1703
512	5	17.894326	0.2528	17.893265	0.2539
	6	18.019977	0.1272	18.014737	0.1324
	7	18.099165	0.0480	18.094732	0.0524
	8	**18.151116**	**0.0040**	**18.152321**	**0.0052**
	9	18.194868	0.0477	18.218433	0.0713
	10	18.231143	0.0840	18.244924	0.0978
	11	18.275571	0.1284	18.284115	0.1370
1024	5	17.977295	0.1698	17.947696	0.1994
	6	18.102537	0.0446	18.038992	0.1081
	7	18.118865	0.0283	18.098850	0.0483
	8	**18.145221**	**0.0019**	**18.150097**	**0.0030**
	9	18.176356	0.0292	18.214874	0.0677
	10	18.202606	0.0555	18.276008	0.1289
	11	18.250397	0.1033	18.294888	0.1477
2048	5	18.007899	0.1392	17.981049	0.1661
	6	18.106753	0.0404	18.056203	0.0909
	7	18.126731	0.0204	18.104529	0.0426
	8	**18.147226**	**0.0001**	**18.146851**	**0.0003**
	9	18.164272	0.0171	18.172111	0.0250
	10	18.193708	0.0466	18.215959	0.0688
	11	18.218186	0.0710	18.260127	0.1130

*The highlighted rows represent the optimal k values for each N.

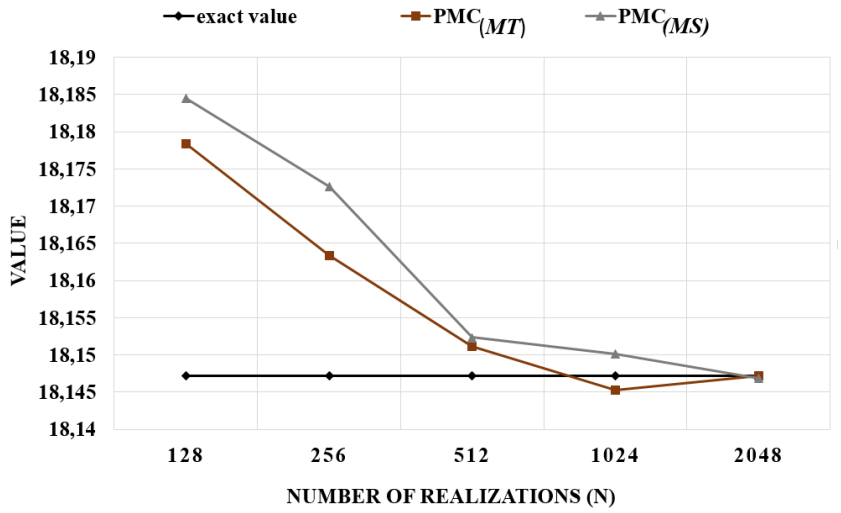


Figure 3.1: Comparison between the exact maximum eigenvalue and the maximum approximate eigenvalue $\lambda_1^{(k)}$ $\lambda_{\max}$ for $PMC_{(MT)}$, $PMC_{(MS)}$ obtained in the balancing cases for different values of N and $k = 8$

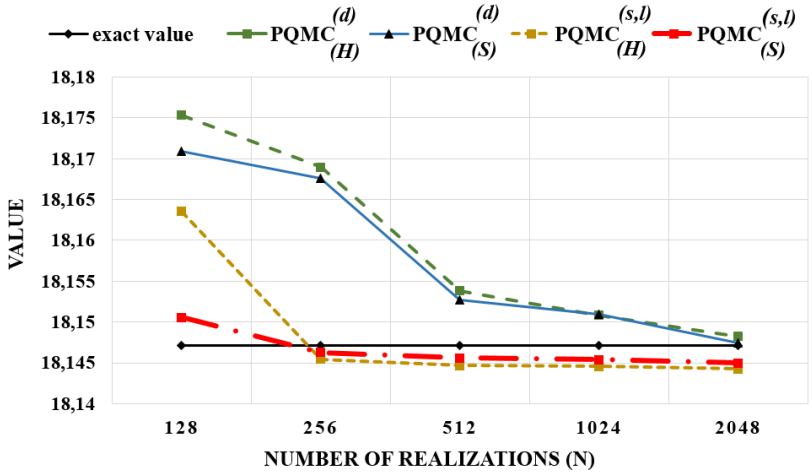


Figure 3.2: $(PQMC^{(d)}_{(H)}, PQMC^{(d)}_{(S)})$ and $(PQMC^{(s,l)}_{(H)}, PQMC^{(s,l)}_{(S)})$. Comparison of the maximum eigenvalue $\lambda_{\max}$ of the correlation matrix with the estimated values $\lambda_1^{(k)}$ obtained when $k = 11$ in the default case and when $k = 13$ in the skip and leap case.

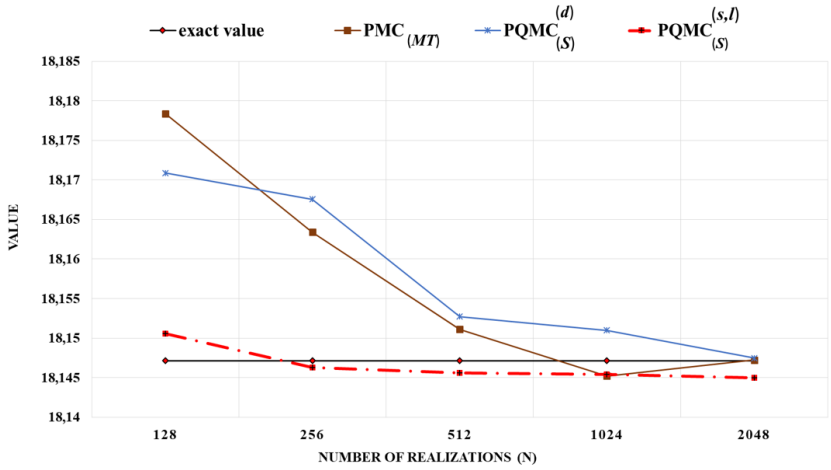


Figure 3.3: Comparison between maximum eigenvalue $\lambda_{\max}$ and approximate eigenvalues $\lambda_1^{(k)}$ obtained at $k = 8$ for $PMC_{(MT)}$, $k = 11$ for $PQMC^{(d)}_{(S)}$ and $k = 13$ for $PQMC^{(s,l)}_{(S)}$ at different values of N.

in absolute error, which stabilizes around $k = 11$ for the default variants $PQMC^{(d)}_{(H)}$ and $PQMC^{(d)}_{(S)}$, and around $k = 13$ for the variants with parameters $PQMC^{(s,l)}_{(H)}$ and $PQMC^{(s,l)}_{(S)}$, indicating reaching a practically optimal balance between the error components. At a fixed k and an increasing N, the algorithms $PQMC^{(d)}_{(H)}$ and $PQMC^{(d)}_{(S)}$ demonstratea monotonic decrease in the errors and stable convergence. In contrast, $PQMC^{(s,l)}_{(H)}$ and $PQMC^{(s,l)}_{(S)}$ show significant improvement for small samples ($N = 128, 256$), but for larger N the error remains almost constant or even increases, which is consistent with the observations in [52] regarding the sensitivity to the parameters *skip* and *leap*.

The graphical comparison in Figure 3.2 confirms the conclusions drawn by illustrating the convergence of the estimates $\lambda_1^{(k)}$ to the exact value λ_1 with an increasing number of realizations N. The algorithms $PQMC^{(d)}_{(S)}$ and $PQMC^{(d)}_{(H)}$ demonstrate stable and smooth convergence, while the variants $PQMC^{(s,l)}_{(H)}$ and $PQMC^{(s,l)}_{(S)}$ show better accuracy for small samples N, but limited improvement for larger samples.

In Figure 3.3, the $PMC_{(MT)}$ and $PQMC^{(d)}_{(S)}$ algorithms stand out with higher accuracy and stability for large N, while for small samples ($N \leq 512$) the use of PQMC algorithms with parameters *skip* and *leap* is more efficient.

Table 3.3 presents estimates of FVE_1 obtained by $PMC_{(MT)}$, $PQMC^{(d)}_{(S)}$ and $PQMC^{(s,l)}_{(S)}$ for the balancing values of k and $N = 256$, 2048, with the reference value being $\text{FVE}_1 = 56.71\%$. The results show that for small

Table 3.2: Results for maximum eigenvalues for $\lambda_{max}^{(k)}$ and absolute error by default scenario and scenario using *skip* and *leap* for different N and k when $\lambda_{max} = 18.14714$

N	k	$\lambda_1^{(k)}$ using $PQMC_{(H)}^{(d)}$	Absolute Error $PQMC_{(H)}^{(d)}$	$\lambda_1^{(k)}$ using $PQMC_{(S)}^{(d)}$	Absolute Error $PQMC_{(S)}^{(d)}$	$\lambda_1^{(k)}$ using $PQMC_{(H)}^{(s,l)}$	Absolute Error $PQMC_{(H)}^{(s,l)}$	$\lambda_1^{(k)}$ using $PQMC_{(S)}^{(s,l)}$	Absolute Error $PQMC_{(S)}^{(s,l)}$
128	8	17.757547	0.3896	17.761379	0.3858	17.672733	0.4744	17.706637	0.4405
	9	17.888100	0.2590	17.888185	0.2590	17.787523	0.3596	17.792723	0.3544
	10	18.016669	0.1305	18.038214	0.1089	17.856741	0.2904	17.859089	0.2881
	11	**18.175307**	**0.0282**	**18.170859**	**0.0237**	17.903166	0.2440	17.914975	0.2322
	12	18.298811	0.1517	18.264832	0.1177	18.036970	0.1102	18.097564	0.0496
	13	18.479146	0.3320	18.474626	0.3275	**18.145462**	**0.0017**	**18.146253**	**0.0009**
	14	18.643362	0.4962	18.639031	0.4919	18.194240	0.0471	18.191902	0.0448
	15	18.712889	0.5657	18.706247	0.5591	18.290732	0.1436	18.290924	0.1438
256	8	17.882593	0.2645	17.883812	0.2633	17.761315	0.3858	17.763949	0.3832
	9	17.994408	0.1527	18.016913	0.1302	17.854804	0.2923	17.867712	0.2794
	10	18.061271	0.0859	18.062487	0.0847	17.936785	0.2104	17.921160	0.2260
	11	**18.168944**	**0.0218**	**18.167556**	**0.0204**	18.036010	0.1111	18.043959	0.1032
	12	18.284126	0.1370	18.251619	0.1045	18.097978	0.0492	18.098070	0.0491
	13	18.482373	0.3352	18.469322	0.3222	**18.145462**	**0.0017**	**18.146253**	**0.0009**
	14	18.545036	0.3979	18.516617	0.3695	18.209384	0.0622	18.185109	0.0380
	15	18.608838	0.4617	18.607262	0.4601	18.289967	0.1428	18.270105	0.1230
512	8	17.927397	0.2197	17.962654	0.1845	17.774098	0.3730	17.778972	0.3682
	9	18.020330	0.1268	18.021557	0.1256	17.846070	0.3011	17.867473	0.2797
	10	18.081105	0.0660	18.081198	0.0659	17.938077	0.2091	17.949995	0.1971
	11	**18.153831**	**0.0067**	**18.152703**	**0.0056**	18.009669	0.1375	18.014807	0.1323
	12	18.263301	0.1162	18.248667	0.1015	18.038078	0.1091	18.038550	0.1086
	13	18.425061	0.2779	18.411903	0.2648	**18.144697**	**0.0024**	**18.145602**	**0.0015**
	14	18.506259	0.3591	18.504204	0.3571	18.204814	0.0577	18.191490	0.0444
	15	18.551586	0.4044	18.546687	0.3995	18.249184	0.1020	18.242947	0.0958
1024	8	17.962214	0.1849	17.978111	0.1690	17.776881	0.3703	17.792702	0.3544
	9	18.035437	0.1117	18.042592	0.1045	17.867701	0.2794	17.887652	0.2595
	10	18.103422	0.0437	18.109582	0.0376	17.980078	0.1671	17.980502	0.1666
	11	**18.150822**	**0.0037**	**18.150986**	**0.0038**	18.010761	0.1364	18.037651	0.1095
	12	18.294487	0.1473	18.284447	0.1373	18.098692	0.0484	18.098718	0.0484
	13	18.385875	0.2387	18.384413	0.2373	**18.144277**	**0.0029**	**18.144964**	**0.0022**
	14	18.446470	0.2993	18.443825	0.2967	18.202841	0.0557	18.203207	0.0561
	15	18.530500	0.3834	18.521017	0.3739	18.236167	0.0890	18.235788	0.0886
2048	8	18.000431	0.1467	18.000619	0.1465	17.787254	0.3599	17.788274	0.3589
	9	18.061446	0.0857	18.064399	0.0827	17.879783	0.2674	17.887915	0.2592
	10	18.108451	0.0387	18.110469	0.0367	17.980078	0.1671	17.980502	0.1666
	11	**18.148212**	**0.0011**	**18.147480**	**0.0003**	18.010923	0.1362	18.040106	0.1070
	12	18.226453	0.0793	18.221684	0.0745	18.118819	0.0283	18.120939	0.0262
	13	18.385443	0.2383	18.379872	0.2327	**18.144277**	**0.0029**	**18.144964**	**0.0022**
	14	18.443228	0.2961	18.435573	0.2884	18.202381	0.0552	18.203555	0.0564
	15	18.509033	0.3619	18.492101	0.3450	18.247648	0.1005	18.243565	0.0964

*The highlighted rows represent the optimal k values for each N

Table 3.3: Approximate values for the fraction of variance explained (FVE_1) obtained at $k = 8$ for $PMC_{(MT)}$, $k = 11$ for $PQMC_{(S)}^{(d)}$ and $k = 13$ for $PQMC_{(S)}^{(s,l)}$ for the correlation matrix $\hat{R}$ with dimension $n = 32$. The reference value is $FVE_1 = 56.71\%$

N	$PMC_{(MT)}$	$PQMC_{(S)}^{(d)}$	$PQMC_{(S)}^{(s,l)}$
256	56.76%	56.77%	56.70%
2048	56.71%	56.71%	56.70%

samples, $PQMC_{(S)}^{(s,l)}$ gives better estimates, while for large N, $PMC_{(MT)}$ and $PQMC_{(S)}^{(d)}$ are more efficient, achieving higher accuracy at lower computational complexity. Finally, the high value of FVE_1 for $n = 32$ indicates the presence of a dominant factor. This means a higher concentration of systematic risk and limited diversification opportunities, as assets respond similarly to market shocks.

3.4.2 Case (ii): correlation matrix with dimension $n = 490$

Table 3.4 presents the numerical results for estimating the maximum eigenvalue $\lambda_1 = \lambda_{\max}$ of a correlation matrix $\hat{R}$ with a high dimension $n = 490$, constructed based on the returns of companies from the index $S\&P500$ for the period 2021–2025 (see the Appendix). Due to incomplete data, 10 companies were excluded from the analysis. Estimation was performed using the algorithms $PMC_{(MT)}$, $PQMC_{(H)}^{(d)}$, and $PQMC_{(S)}^{(d)}$, for different values of the number of transitions k and the number of realizations N, and the corresponding absolute errors were also analyzed. The estimation was performed using the *almost optimal* PMC algorithm $PMC_{(MT)}$

and the *almost optimal* PQMC algorithms $PQMC^{(d)}_{(H)}$ and $PQMC^{(d)}_{(S)}$, using Halton and Sobol sequences with default settings. The results show that the parameters k and N have a significant impact on the precision of the estimations, with the balancing values of the number of transitions being $k = 8$ for $PMC_{(MT)}$ and $k = 11$ for $PQMC^{(d)}_{(H)}$ and $PQMC^{(d)}_{(S)}$, despite the significantly larger dimensionality compared to the case $n = 32$.

Table 3.4: Results for maximum eigenvalues for $\lambda^{(k)}_{max}$ and absolute error for $PMC_{(MT)}, PQMC^{(d)}_{(H)}$ and $PQMC^{(d)}_{(S)}$ at different N and k when $\lambda_{max} = 201.090512$

N	k	$\lambda_1^{(k)}$ using $PMC_{(MT)}$	Absolute Error $PMC_{(MT)}$	k	$\lambda_1^{(k)}$ using $PQMC^{(d)}_{(H)}$	Absolute Error $PQMC^{(d)}_{(H)}$	$\lambda_1^{(k)}$ using $PQMC^{(d)}_{(S)}$	Absolute Error $PQMC^{(d)}_{(S)}$
512	6	191.261222	9.8293	8	192.052259	9.0383	192.056796	9.0337
	7	197.764391	3.3261	9	193.305250	7.7853	194.4876692	6.6028
	8	**203.030089**	**1.9396**	10	196.545330	4.5452	196.561636	4.5289
	9	206.001210	4.9107	**11**	**202.016871**	**0.9264**	**201.830255**	**0.7397**
	10	209.202619	8.1121	12	207.216480	6.1260	206.994716	5.9042
1024	6	194.244715	6.8458	8	191.604757	9.4858	191.662089	9.4284
	7	199.671479	1.4190	9	194.355045	6.7355	194.443329	6.6472
	8	**202.103664**	**1.0132**	10	198.362863	2.7276	196.623242	4.4673
	9	204.706063	3.6156	**11**	**201.526659**	**0.4361**	**201.467671**	**0.3772**
	10	211.940453	10.8499	12	204.493635	3.4031	204.718275	3.6278
2048	6	196.531375	4.5591	8	191.522259	9.5683	191.737033	9.3535
	7	199.092487	1.9980	9	194.216871	6.8736	194.383618	6.7069
	8	**201.462168**	**0.3717**	10	198.552479	2.5380	198.866204	2.2243
	9	204.787620	3.6971	**11**	**201.267671**	**0.1772**	**201.199260**	**0.1087**
	10	206.264686	5.1942	12	207.590516	6.5000	206.670141	5.5796
4096	6	195.762474	5.3280	8	194.293635	6.7969	195.846272	6.2442
	7	197.402088	3.6884	9	198.498616	2.5919	198.498988	2.5915
	8	**201.154640**	**0.0641**	10	199.459470	1.6310	199.802438	1.2881
	9	202.887637	1.7971	**11**	**201.083321**	**0.0072**	**201.091681**	**0.0012**
	10	207.343376	6.2529	12	206.448996	5.3585	205.624451	4.5339

*The highlighted rows represent the optimal k values for each N

The results show that the optimal balance between systematic and stochastic error is achieved at $k = 8$ for $PMC_{(MT)}$ and $k = 11$ for $PQMC^{(d)}_{(H)}$ and $PQMC^{(d)}_{(S)}$, regardless of the larger dimensionality of the matrix. At a fixed k, a monotonic decrease in the absolute error is observed with increasing number of realizations N, with the minimum errors noted in Table 3.4. Figure 3.4 illustrates that all algorithms demonstrate stable convergence to the reference value $\lambda_{\max}$, with the PQMC variants $PQMC^{(d)}_{(H)}$ and $PQMC^{(d)}_{(S)}$ showing faster and smoother convergence compared to $PMC_{(MT)}$. The estimates obtained for λ_1 allow for a precise calculation of FVE_1 using formula (3.12), the results are presented in Table 3.5.

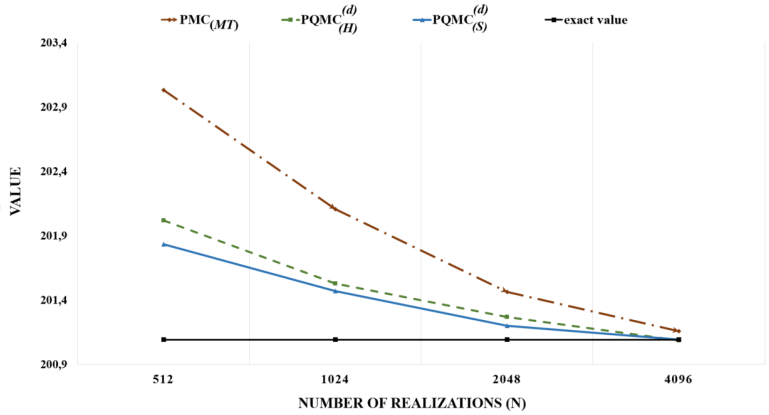


Figure 3.4: Comparison between the exact maximum eigenvalue ($\lambda_{\max}$) and the maximum approximate eigenvalue ($\lambda_1^{(k)}$) for $PMC_{(MT)}$, $PQMC^{(d)}_{(H)}, PQMC^{(d)}_{(S)}$, obtained when $k = 8$ in the case of $PMC_{(MT)}$ and $k = 11$ in the case of $PQMC^{(d)}_{(*)}$ and different values of N

Table 3.5: Approximate values for the fraction of variance explained (FVE_1) obtained at $k = 8$ for $PMC_{(MT)}$ and at $k = 11$ for $PQMC^{(d)}_{(H)}$ and $PQMC^{(d}_{(S)}$ for the correlation matrix $\hat{R}$ with dimension $n = 490$. The reference value is $\text{FVE}_1 = 41.04\%$

N	$PMC_{(MT)}$	$PQMC^{(d)}_{(H)}$	$PQMC^{(d)}_{(S)}$
1024	41.25%	41.13%	41.12%
2048	41.11%	41.08%	41.06%
4096	41.05%	41.04%	41.04%

The estimates obtained for λ_1 by $PQMC^{(d)}_{(H)}$ and $PQMC^{(d)}_{(S)}$ allow a more precise calculation of the fraction of the explained variation FVE_1 by formula (3.12). Table 3.5 presents the corresponding results obtained at the balancing values $k = 8$ and $k = 11$, with the reference value being $\text{FVE}_1 = 41.04\%$. Data show that when N increases, the use of the PQMC algorithms $PQMC^{(d)}_{(H)}$ and $PQMC^{(d)}_{(S)}$ is preferable to $PMC_{(MT)}$ due to higher precision at comparable computational complexity.
The value $\text{FVE}_1 \approx 41\%$ for the correlation matrix with dimension $n = 490$ shows that the variation is not concentrated in the first principal component but is distributed among multiple factors. This indicates a more complex structure of dependencies between assets and suggests a higher potential for diversification. At the same time, this result requires the use of multifactor models to adequately describe market risk, since single-factor approaches would be insufficient to capture the observed dynamics.

3.5 Summary

The results confirm the practical applicability and computational efficiency of the *almost optimal* stochastic algorithms for estimating the maximum eigenvalue of correlation matrices in market risk analysis. The analyzed matrices, with dimensions $n = 32$ and $n = 490$, are constructed based on data from *Portfolio Visualizer* and *Yahoo Finance* (see Appendix), where the maximum eigenvalue is interpreted as an indicator of the dominant market factor. Analysis of the correlation matrices shows that the largest eigenvalue, λ_1, is clearly interpreted as a measure of the presence and strength of a dominant common market factor. Through the corresponding fraction of variance explained FVE_1, a quantitative assessment is obtained for both the level of systematic risk and the limitations of effective portfolio diversification.
Numerical experiments for the case $n = 32$ show that, for *almost optimal* PMC algorithms, the balance between stochastic and systematic error is achieved at $k = 8$. For *almost optimal* PQMC algorithms that use scrambled Sobol and Halton sequences with default settings, this balance is reached at $k = 11$. In the case when applying the *skip* and *leap* operators, it is achieved at $k = 13$. Furthermore, as the number of realizations N increases, the absolute error decreases monotonically for both PMC and PQMC algorithms with default settings, confirming their stable convergence behaviour.
A significant result is that, for high-dimensional matrices ($n = 490$), the *almost optimal* PQMC algorithms with default settings demonstrate better convergence and higher accuracy compared to the *almost optimal* PMC algorithms. At the same time, the use of *skip* and *leap* operators is effective mainly for small sample sizes N. In contrast, for larger samples, their advantage diminishes and does not guarantee a further improvement in accuracy. Some of the results presented have been published in [38].
In conclusion, the developed *almost optimal* stochastic power algorithms represent a reliable tool for the numerical estimation of spectral characteristics of correlation matrices. This enables a deeper analysis of systematic risk, collective asset dynamics, and diversification efficiency, while also providing a foundation for future applications in financial modeling, portfolio management, and decision support in high-dimensional problems.

Conclusion

This dissertation is devoted to the development, analysis, and application of stochastic numerical methods, namely Monte Carlo (MC) and randomized Quasi-Monte Carlo (QMC) methods for estimating extreme eigenvalues of symmetric matrices and their application to practical problems related to risk assessment and investment portfolio optimization. The main objective is to construct a stable, computationally efficient methodological framework that maintains a controllable balance between systematic and stochastic errors and applies to high-dimensional problems.

Within the scope of the research, the Power (Resolvent) Monte Carlo method and the randomized Power (Resolvent) Quasi-Monte Carlo method for estimating extreme eigenvalues are theoretically justified and investigated. A significant result is the refinement of the construction of random variables when using an almost optimal transition density in the Markov chain, as well as the identification of classes of symmetric matrices for which this construction is simplified. On this basis, almost optimal algorithms (Power and Resolvent MC and QMC) are developed and presented in pseudocode, along with estimates of their computational complexity and conditions for balancing statistical and systematic errors. Theoretical arguments and experimental results confirm that the proposed almost optimal constructions lead to reduced variance and improved accuracy at equal or lower computational cost compared to classical stochastic analogues.

The experimental validation is performed using both pseudo-random number generators (MT and MS) and low-discrepancy sequences (Sobol and Halton sequences), including their scrambled variants. Numerical experiments demonstrate a measurable impact of the choice of generator and sequence type on the accuracy and stability of the estimates. In the tests considered, the MT pseudorandom number generator outperforms the MS generator, while scrambled Sobol sequences outperform scrambled Halton sequences. It is also established that, in order to achieve a comparable balance of errors, the randomized Power (Resolvent) QMC algorithm may require a slightly larger number of transitions in the Markov chain, which is compensated by improved convergence under limited computational resources.

The developed algorithms are applied to a financial mathematics problem related to managing the risk of an investment portfolio. The maximum eigenvalue of the asset correlation matrix is used as an indicator of risk concentration, and its estimation is performed using the proposed MC and QMC algorithms, including additional randomization techniques such as *skip* and *leap* applied to scrambled low-discrepancy sequences (Sobol and Halton sequences).

In conclusion, the dissertation demonstrates that applying the proposed algorithms for spectral estimation, combined with targeted error balancing, yields higher accuracy, stability, and computational efficiency. Future research directions are also outlined, including extensions to robust models, dynamic covariance structures, and further computational optimizations for large-scale sparse symmetric matrices with dimensions on the order of millions.

List of Publications on the Dissertation

The following publications present results from the dissertation:

1. **Gurova, S.-M.**, Karaivanova, A., *Quasi-Monte Carlo Algorithms for Eigenvalue Problems, 4th International Conference Numerical Methods for Scientific Computations and Advanced Applications*, NMSCAA'24, 18-22, (**2024**) (short communication)
   `https://parallel.bas.bg/~elilkova/nmscaa24.pdf`

2. **Gurova, S.-M.**, Atanassov, E., Karaivanova, A., *A Resolvent Quasi-Monte Carlo Method for Estimating the Minimum Eigenvalues Using the Error Balancing*, In: Lirkov, I., Margenov, S. (eds), Large-Scale Scientific Computing, LSSC'23, **LNCS**, vol. **13952**, 394-403, (**2024**), (SJR:0.352, 2024)
   `https://doi.org/10.1007/978-3-031-56208-2_40`

3. **Gurova, S.-M.**, Gurov, T., Karaivanova, A., *On the Stochastic Power Algorithms for Estimating the Maximum Eigenvalue of Symmetric Matrices*, **Contemp. Math.**, Universal Wiser Publisher Pte. Ltd, **6(5)**: 7223-49,(**2025**) `doi.org/10.37256/cm.6520257781` (**IF:2.5**, 2025, **WoS: Q1**, `https://wos-journal.info/journalid/23187`)

4. **Gurova, S.-M.**, Gurov, T., Karaivanova, A., *Eigenvalue Estimation in Portfolio Risk: The Role of Skipping and Leaping in Sobol and Halton Sequences*, In: Lirkov, I., Margenov, S. (eds), Large-Scale Scientific Computing, LSSC'25, **LNCS**, **16061**, (accepted)

Approbation of the Results

The results included in the dissertation have been reported at seminars of the section "Scalable Algorithms and Cybersecurity with the Center for High Performance Computing" at IICT-BAS, as well as at international conferences. The following reports related to the topic of the dissertation have been presented:

1. Gurova, S.-M., Monte Carlo Method for Estimating Eigenvalues Using Error Balancing, The 13th International Conference on Large-Scale Scientific Computations, LSSC'21, 07-11.06.2021, Sozopol, Bulgaria. https://parallel.bas.bg/Conferences/SciCom21/program.html
2. Gurova, S.-M., A Quasi-Monte Carlo method for estimation of eigenvalues using error balancing, The 15th International Conference on Monte Carlo and Quasi-Monte Carlo methods in Scientific Computing, MCQMC'22, 17-22.07.2022, Linz, Austria. https://www.ricam.oeaw.ac.at/events/conferences/mcqmc2022/schedule/MCQMC2022_book_final_version.pdf
3. Gurova, S.-M., Power Monte Carlo method using randomized low discrepancy sequences, the 17th Annual Meeting of the Bulgarian Section of SIAM, 20-22.12.2022, BGSIAM'22, Sofia, Bulgaria. http://www.math.bas.bg/bgsiam/docs/bgsiam_2022_program.pdf
4. Gurova, S.-M., A Resolvent Quasi-Monte Carlo Method for Estimating the Minimum Eigenvalues Using the Error Balancing, The 14th International Conference on Large-Scale Scientific Computations, LSSC'23, 05-09.06.2023, Sozopol, Bulgaria. https://parallel.bas.bg/~elilkova/lssc23.pdf#page=17
5. Gurova, S.-M., Quasi-Monte Carlo Algorithms for Eigenvalue Problems, Fourth International Conference Numerical Methods for Scientific Computations and Advanced Applications, NMSCAA'24, 17-21.06.2024, Sozopol, Bulgaria. https://parallel.bas.bg/Conferences/nmscaa24/program.html

The articles present results obtained within the framework of one international and three national scientific projects, one of which is divided into two phases, namely:

1. **International Scientific Project**
   - New Scalable Algorithms Using Monte Carlo and Quasi-Monte Carlo Methods and Their Application in the Field of Machine Learning, funded by CAF America, 2021-2024, head: Prof. Emanuil Atanasov, PhD.
2. **National Scientific Projects**
   - "Center of Excellence in Informatics and Information and Communication Technologies" (phase 1) under contract BG05M2OP001-1.001-0003, funded by the Operational Program "Science and Education for Smart Growth" 2014-2020, co-financed by the European Union through the European Structural and Investment Funds, head: Corr. Mem. Svetozar Margenov.
   - "National Geoinformation Center (NGIC) for monitoring, assessment and forecasting of natural and anthropogenic risks and disasters" object of the "National Roadmap for Scientific Infrastructure 2020-2027", funded by the Ministry of Education and Science under the contracts: D01-321/30.11.2023 and D01-164/28.07.2022, head: Assoc. Prof. Petya Trifonova.
   - "National Center for High-Performance and Distributed Computing" (NCHDC) object of the "National Roadmap for Scientific Infrastructure 2020-2027", funded by the Ministry of Education and Science under the contracts: D01-98/26.06.2025, D01-325/01.12.2023, head: Prof. Aneta Karaivanova.
   - "Center for Excellence in Informatics and Information and Communication Technologies" (phase 2) under contract BG16RFPR002-1.014-0018-C01, funded under the Research, Innovation and Digitalisation for Smart Transformation Programme 2021-2027 and co-financed by the European Union, head: Corr. Mem. Svetozar Margenov.

Major Scientific and Applied Contributions

The obtained scientific and applied contributions fully correspond to the stated objectives and tasks of the dissertation. They directly reflect the theoretical justification, development, and experimental investigation of Power MC/QMC algorithms and Resolvent MC/QMC algorithms for estimating extreme eigenvalues of symmetric matrices. Furthermore, the contributions are validated through a real-world application in financial mathematics, namely the assessment of market risk in a portfolio of global assets.

1. The main scientific contributions of the dissertation are:

   - The Power (Resolvent) Monte Carlo method and the randomized Power (Resolvent) Quasi-Monte Carlo method for estimating extreme eigenvalues of symmetric matrices are theoretically justified and investigated. The construction of the random variables $\theta^{(k)}$ and $\theta^{(k-1)}$ is refined when using an almost optimal transition density in the Markov chain. Classes of symmetric matrices are identified for which this construction is simplified. Theoretical estimates are derived for the relationship between the degree of the resolvent matrix and the length of the Markov chain, as a function of the acceleration parameter and the matrix norm.
   - The almost optimal Power MC/QMC and almost optimal Resolvent MC/QMC algorithms are developed based on the proposed refined construction of the random variables. These algorithms are presented in pseudocode form. Estimates of their computational complexity are provided, along with conditions for balancing stochastic and systematic errors. It is demonstrated that the proposed algorithms lead to variance reduction compared to classical stochastic approaches.
   - A practical problem from financial mathematics is proposed, related to the assessment of market risk in investment portfolios. The constructed correlation matrix of the portfolio is used to estimate the maximum eigenvalue, which serves as an indicator of risk concentration. The estimation is performed using the almost optimal Power MC and Power QMC algorithms developed in Chapter 1, with the QMC algorithm further enhanced by the parameters *skip* and *leap*.

2. The main applied contributions of the dissertation are:

   - The proposed almost optimal Power MC algorithms are implemented using MT and MS pseudo-random number generators, while the Power QMC algorithms are implemented using scrambled Sobol and Halton sequences. Numerical experiments for estimating the maximum eigenvalue of large dense symmetric matrices demonstrate the superiority of the almost optimal algorithms over their classical counterparts in terms of both accuracy and computational efficiency.
   - The balance between stochastic and systematic error is numerically investigated and shown to depend significantly on the number of transitions k in the Markov chain and the number of realizations N of the random variables $\theta^{(k)}$ and $\theta^{(k-1)}$. The results indicate that QMC algorithms require approximately two or three additional steps in the Markov chain compared to MC algorithms. The choice of pseudo-random number generator or low-discrepancy sequence has a measurable effect on accuracy and stability; in the experiments conducted, the MT generator outperforms MS, while Sobol sequences outperform Halton sequences.
   - The almost optimal Resolvent MC algorithm is implemented using the MT pseudo-random number generator, while the almost optimal Resolvent QMC algorithm is implemented using a scrambled Sobol sequence via the BRODA Sobol RSG generator. Numerical experiments conducted on an HPC cluster with NVIDIA Tesla V100 (32 GB) GPUs to estimate the minimum eigenvalue show that the balance between stochastic and systematic error depends on the number of Markov chain transitions k, the number of realizations N, the degree m of the resolvent matrix and the acceleration parameter q. The results obtained using randomized Sobol sequences and the MT generator demonstrate the same order of convergence. A key factor is the ability to determine a constant that separates the minimum eigenvalue from zero.
   - Numerical experiments are conducted to estimate the maximum eigenvalue of two correlation matrices used as indicators of market risk concentration. The first matrix is constructed based on the returns of 32 global assets, while the second uses returns from 490 companies from the $S\&P500$ index over specific time periods (see Appendix). The estimation is performed using the almost optimal Power MC algorithm with MT/MS generators and the almost optimal Power QMC algorithm, both in default settings and with additional tuning using the *skip* and *leap* parameters for scrambled Sobol and Halton sequences.

Appendix

The numerical experiments are carried out using generated symmetric matrices (Chapter 1, Chapter 2) and real financial data (Chapter 3). The symmetric matrices of sizes 100 and 500 used in Chapter 1 are generated using the MATLAB software environment, while those of sizes 500 and 1000 in Chapter 2 are part of an algorithmic implementation developed in the C++ programming language.
The financial data used to construct the correlation matrix of dimension $n = 32$ in Chapter 3 are obtained from the web platform *Portfolio Visualizer* (`www.portfoliovisualizer.com`). The studied time horizon covers the period from January 2007 to March 2024 and is based on real market indicators. Based on this empirical data, an investment portfolio is constructed. The portfolio consists of thirty-two global assets, classified according to their investment type as follows:

1. **Eighteen equities** – "US Stock Market", "US Large Cap Value", "US Large Cap Growth", "US Mid Cap", "US Mid Cap Value", "US Mid Cap Growth", "US Small Cap Value", "US Small Cap Growth", "US Large Cap", "US Small Cap", "US Micro Cap", "Global ex-US Stock Market", "European Stocks", "Pacific Stocks", "Emerging Markets", "Intl Developed ex-US Market", "International ex-US Small Cap", "International ex-US Value";

2. **Nine bonds** – "Short Term Treasury", "Intermediate Term Treasury", "10-year Treasury", "Long Term Treasury", "Total US Bond Market", "Global Bonds (USD Hedged)", "Short-Term Investment Grade", "TIPS (Treasury Inflation-Protected Securities)", "Corporate Bonds";

3. **Four alternative investments** – "REIT (Real Estate Investment Trusts)", "Gold", "Precious Metals", "Commodities";

4. **One cash asset & equivalents** – "Cash".

The financial data used to construct the correlation matrix of dimension $n = 490$ in Chapter 3 consist of the returns of 490 companies from the $S\&P500$ ($Standard\&Poor's$ 500), an index measuring the performance of the U.S. stock market, over 5 years from 2021 to 2025. The return data were downloaded from *Yahoo Finance* (`https://finance.yahoo.com/`) using the *yFinance* library, available via the *PyPI* repository (`https://pypi.org/project/yfinance/`). This library enables automated retrieval of historical price series and market indicators through an interface to the *Yahoo Finance* website, allowing programmatic data extraction for specific financial instruments over a given time interval and their subsequent processing in an analytical environment.

1. The generated symmetric matrices of sizes 100 and 500 used in Chapter 1 are published on the **GitHub** platform and are available at:

   - `https://github.com/smgurova/Symmetric-matrices_chapter-1.git`

2. The financial report provided by *Portfolio Visualizer* is available on **GitHub** at:

   - `https://github.com/smgurova/AssetAllocation.git`

3. The correlation matrix of the thirty-two global assets used in the numerical experiments in Chapter 3 is available on **GitHub** at:

   - `https://github.com/smgurova/correlation-matrix_chapter-4.git`

4. The return data of 490 companies from the $S\&P500$ ($Standard\&Poor's$ 500) for the period 2021–2025, along with the resulting correlation matrix used in the numerical experiments in Chapter 3, are available on **GitHub** at:

   - `https://github.com/smgurova/Data-S-P500.git`

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