Discrepancy Bounds for Deterministic Acceptance-Rejection Samplers

Author:
Zhu, Houying

Publication Date:
2016

DOI:
https://doi.org/10.26190/unsworks/19043

License:
https://creativecommons.org/licenses/by-nc-nd/3.0/au/
Link to license to see what you are allowed to do with this resource.

Downloaded from http://hdl.handle.net/1959.4/56305 in https://unsworks.unsw.edu.au on 2024-04-29

Discrepancy Bounds for Deterministic Acceptance-Rejection Samplers

Houying Zhu

A thesis in fulfilment of the requirements for the degree of

Doctor of Philosophy

School of Mathematics and Statistics

Faculty of Science

The University of New South Wales, Australia

31 March 2016

PLEASE TYPE

THE UNIVERSITY OF NEW SOUTH WALES
Thesis/Dissertation Sheet

Surname or Family name: **Zhu**

First name: **Houying** Other name/s:

Abbreviation for degree as given in the University calendar: **PhD**

School: **School of Mathematics and Statistics** Faculty: **Faculty of Science**

Title: **Discrepancy bounds for deterministic acceptance-rejection samplers**

Abstract 350 words maximum: (PLEASE TYPE)

The Monte Carlo method is one of the widely used numerical methods for simulating probability distributions. Its convergence rate is independent of the dimension but slow. Quasi-Monte Carlo methods, which can be seen as a deterministic version of Monte Carlo methods, have been developed to improve the convergence rate to achieve greater accuracy, which partially depends on generating samples with small discrepancy. Putting the quasi-Monte Carlo idea into statistical sampling is a good way to improve the convergence rate and widen practical applications.

In this thesis we focus on constructing low-discrepancy point sets with respect to non-uniform target measures using the acceptance-rejection sampler. We consider the acceptance-rejection samplers based on different driver sequences. The driver sequence is chosen such that the discrepancy between the empirical distribution and the target distribution is small. Hence digital nets, stratified inputs and lattice point sets are used for this purpose. The central contribution in this work is the establishment of discrepancy bounds for samples generated by acceptance-rejection samplers. Together with a Koksma-Hlawka type inequality, we obtain an improvement of the numerical integration error for non-uniform measures.

Furthermore we introduce a quality criterion for measuring the goodness of driver sequences in the acceptance-rejection method. Explicit constructions of driver sequences yield a convergence order beyond plain Monte Carlo for samples generated by the deterministic acceptance-rejection samplers in dimension one.

The proposed algorithms are numerically tested and compared with the standard acceptance-rejection algorithm using pseudo-random inputs. The empirical evidence confirms that adapting low-discrepancy sequences in the acceptance-rejection sampler outperforms the original algorithm.

Declaration relating to disposition of project thesis/dissertation

I hereby grant to the University of New South Wales or its agents the right to archive and to make available my thesis or dissertation in whole or in part in the University libraries in all forms of media, now or here after known, subject to the provisions of the Copyright Act 1968. I retain all property rights, such as patent rights. I also retain the right to use in future works (such as articles or books) all or part of this thesis or dissertation.

I also authorise University Microfilms to use the 350 word abstract of my thesis in Dissertation Abstracts International (this is applicable to doctoral theses only).

The University recognises that there may be exceptional circumstances requiring restrictions on copying or conditions on use. Requests for restriction for a period of up to 2 years must be made in writing. Requests for a longer period of restriction may be considered in exceptional circumstances and require the approval of the Dean of Graduate Research.

FOR OFFICE USE ONLY Date of completion of requirements for Award:

THIS SHEET IS TO BE GLUED TO THE INSIDE FRONT COVER OF THE THESIS

ORIGINALITY STATEMENT

'I hereby declare that this submission is my own work and to the best of my knowledge it contains no materials previously published or written by another person, or substantial proportions of material which have been accepted for the award of any other degree or diploma at UNSW or any other educational institution, except where due acknowledgement is made in the thesis. Any contribution made to the research by others, with whom I have worked at UNSW or elsewhere, is explicitly acknowledged in the thesis. I also declare that the intellectual content of this thesis is the product of my own work, except to the extent that assistance from others in the project's design and conception or in style, presentation and linguistic expression is acknowledged.'

Signed ……..

Date ……..

COPYRIGHT STATEMENT

'I hereby grant the University of New South Wales or its agents the right to archive and to make available my thesis or dissertation in whole or part in the University libraries in all forms of media, now or here after known, subject to the provisions of the Copyright Act 1968. I retain all proprietary rights, such as patent rights. I also retain the right to use in future works (such as articles or books) all or part of this thesis or dissertation.
I also authorise University Microfilms to use the 350 word abstract of my thesis in Dissertation Abstract International (this is applicable to doctoral theses only).
I have either used no substantial portions of copyright material in my thesis or I have obtained permission to use copyright material; where permission has not been granted I have applied/will apply for a partial restriction of the digital copy of my thesis or dissertation.'

Signed …….....

Date …….....

AUTHENTICITY STATEMENT

'I certify that the Library deposit digital copy is a direct equivalent of the final officially approved version of my thesis. No emendation of content has occurred and if there are any minor variations in formatting, they are the result of the conversion to digital format.'

Signed …….....

Date …….....

Abstract

The Monte Carlo method is one of the widely used numerical methods for simulating probability distributions. Its convergence rate is independent of the dimension but slow. Quasi-Monte Carlo methods, which can be seen as a deterministic version of Monte Carlo methods, have been developed to improve the convergence rate to achieve greater accuracy, which partially depends on generating samples with small discrepancy. Putting the quasi-Monte Carlo idea into statistical sampling is a good way to improve the convergence rate and widen practical applications.

In this thesis we focus on constructing low-discrepancy point sets with respect to non-uniform target measures using the acceptance-rejection sampler. We consider the acceptance-rejection samplers based on different driver sequences. The driver sequence is chosen such that the discrepancy between the empirical distribution and the target distribution is small. Hence digital nets, stratified inputs and lattice point sets are used for this purpose. The central contribution in this work is the establishment of discrepancy bounds for samples generated by acceptance-rejection samplers. Together with a Koksma-Hlawka type inequality, we obtain an improvement of the numerical integration error for non-uniform measures.

Furthermore we introduce a quality criterion for measuring the goodness of driver sequences in the acceptance-rejection method. Explicit constructions of driver sequences yield a convergence order beyond plain Monte Carlo for samples generated by the deterministic acceptance-rejection samplers in dimension one.

The proposed algorithms are numerically tested and compared with the standard acceptance-rejection algorithm using pseudo-random inputs. The empirical evidence confirms that adapting low-discrepancy sequences in the acceptance-rejection

sampler outperforms the original algorithm.

Acknowledgements

I would like to use this opportunity to thank some of the people who have helped me throughout my PhD program and prepare this thesis.

Foremost I would like to express my sincere gratitude to my main supervisor Josef Dick for the continuous support of my Ph.D program, especially for his patience, but also for his profound knowledge, sound advices and insightful comments at different stages of my study. His guidance helped me during the time of my research and the writing of this thesis. I could not imagine a better supervisor with such incredible support and encouragement. I would also like to extend my gratitude to my co-supervisor, Frances Kuo, for always being supportive, a great mentor and a thoughtful friend. In particular I want to thank Frances for making me aware of excellent opportunities, such as conferences and special programs.

Thanks also to my collaborator Daniel Rudolf for the series of lectures about Markov chain Monte Carlo he gave at the very beginning of my PhD, for his hospitality during my visit to Friedrich Schiller University Jena, Germany, in Apr. 2014.

Thanks to Peter Krizer for inviting me to visit Johannes Kepler University Linz, Austria in Dec. 2015. Thanks to Peter Krizer and Friedrich Pillichshammer for their hospitality during my visit.

Thanks to the quasi-Monte Carlo community around the world for organizing excellent conferences, workshops and semester programs. I certainly benefit a lot from presenting our work at those events. Special thanks goes to Fred Hickernell, Pierre L'Ecuyer, Christiane Lemieux, Art Owen, Mario Ullrich, Xiaoqun Wang, for their valuable advice on my topic during conference coffee-break discussions and email conversations.

I would also like to thank my family for their encouragement and understanding during all stages of my education. With greatest thanks to my beloved husband, Yuguang Wang, for being the best friend and a great company and collaborator during our academic journey.

Finally, I would like to acknowledge the financial support for my PhD study:

- Tuition Fee Scholarship from the UNSW Australia for my PhD research program.
- The partial support from Postgraduate Research Support Scheme (PRSS) from the Graduate Research School of UNSW to fund my conference trip to MCQMC 2014 in Belgium.
- The support from the Institute for Computational and Experimental Research in Mathematics (ICERM), Brown University, for participating in the semester program on "High-dimensional Approximation" in Fall 2014, Providence, US.
- I gratefully acknowledge Josef Dick, Frances Kuo and Ian Sloan and the Australian Research Council (ARC) for supporting many of my conference trips.

Contents

List of Figures

List of Tables

Chapter 1

Introduction

1.1 Scope of research

Numerical integration is a common computational problem occurring in many areas of science, such as statistics, financial mathematics and computational physics, where one has to compute some integral, for instance an expectation value, which cannot be done analytically. The Monte Carlo (MC) method is one of the widely used numerical methods for simulating probability distributions. Although the convergence rate of Monte Carlo integration is independent from the dimension, it remains at $N^{-1/2}$ for arbitrary dimension, assuming that the variance of the integrand is bounded independent of the dimension. Note that although Monte Carlo commonly assumes that true random numbers are used as inputs, in practice usually one uses deterministic inputs, called pseudo-random numbers, which are designed to mimic true random numbers.

Quasi-Monte Carlo (QMC) methods, which can be seen as a deterministic version of Monte Carlo methods, have been developed to improve the convergence rate to achieve greater accuracy. QMC techniques draw attention from both theoretical and practical aspects. The tools used to develop and analyse quasi-Monte Carlo methods are very different from those in plain Monte Carlo, but randomization techniques applied to deterministic constructions in QMC, often known as random-

ized quasi-Monte Carlo (RQMC) methods, allow us to combine the strengths of these two methods [53, 56, 60]. In addition, Markov chain Monte Carlo (MCMC) methods can be used if only partial information about the target density is available. Thus MCMC can widen the applications where MC type sampling can be used [13, 54]. Therefore combining the methods of QMC or RQMC and MCMC might be a good way to overcome the shortcomings of ordinary Monte Carlo sampling. We call such a method Markov chain quasi-Monte Carlo (MCQMC).

The crucial part for doing numerical integration is determining the quadrature points. Choosing them randomly leads to the Monte Carlo method, whereas deterministically designed points fall into the area of quasi-Monte Carlo rules. Our interest is in deterministic constructions with the goal to obtain a better rate of convergence. The quality measure used in the analysis of samples generated by the MCQMC approach in this thesis is the so-called discrepancy. The concept of discrepancy is introduced to measure the deviation of a sequence from the uniform distribution [22, 23]. With a reasonable generalization, the definition of discrepancy can be extended to arbitrary Borel measures. The aim is then to construct good point sets which have small discrepancy with respect to certain measures.

The reason we are interested in the discrepancy of the samples can be explained by considering numerical integration. The celebrated Koksma-Hlawka inequality roughly states that if one uses the average of empirical function values at some quadrature points to approximate an integral, then the integration error is bounded by a product of two terms, namely, the discrepancy of the quadrature points and the variation of the integrand. We can see that for a fixed integrand, the approximation error depends on how small the discrepancy of the quadrature point set is. Additionally, if we analyse the worst-case integration error, for a given function space and norm, the worst-case error then only depends on the quadrature point set. Further this worst-case error can be related to the discrepancy of the point set for certain reproducing kernel Hilbert spaces [23, 40, 62].

Classical discrepancy theory deals with distributing N points in the s-dimensional unit cube as evenly as possible. If the target distribution is the uniform distribu-

tion in the unit cube $[0,1]^s$, then there are known constructions of low-discrepancy sequences, such us digital nets and lattice methods [22, 23, 60]. But much less is known for non-uniform measures, besides applying the inversion method and special transformations for standard distributions to low-discrepancy point sets and sequences with respect to the uniform distribution. Regarding sampling from non-uniform distributions beyond the inversion method, there are classical principles from statistics, namely acceptance-rejection, weighting and composition, which can be used in conjunction with statistical samplers [18, 42].

Recently an existence result concerning low-discrepancy point sets regarding non-uniform measures was given by Aistleitner and Dick in [3]. They proved that there exists a sample set for arbitrary Borel measures whose discrepancy is of order $(\log N)^{(3s+1)/2}/N$. This result is based on a probabilistic argument. However, in general how to explicitly construct point sets which achieve a convergence rate for discrepancy beyond $N^{-1/s}$ for non-uniform measures is not known. Motivated by these facts, this thesis is concerned with constructing low-discrepancy point sets with respect to non-uniform target measures. We use the discrepancy to measure the quality of samples obtained by our statistical samplers, which are based on explicit constructions of the initial samples. Precise details are given in the following chapters.

1.2 Literature review

Using a deterministic point set as the driver sequence in the MCMC procedure, known as Markov chain quasi-Monte Carlo (MCQMC) algorithm, shows potential to improve the convergence rate. Recently several results in this direction have been achieved, see for instance [15, 16, 79, 80] and references therein. We briefly review some results.

Tribble and Owen [80] proved a consistency result for MCMC estimation for finite state spaces. A construction of weakly completely uniformly distributed (WCUD) sequences is also proposed. As a sequel to the work of Tribble, Chen

[15] and Chen, Dick and Owen [16] demonstrated that MCQMC algorithms, using a completely uniformly distributed sequence as the driver sequence, give a consistent result under certain assumptions on the update function and Markov chain. Further, Chen [15] also showed that MCQMC can achieve a convergence rate of $O(N^{-1+\delta})$ for any $\delta > 0$ under certain stronger assumptions, but he only showed the existence of a driver sequence. More information on completely uniformly distributed sequences can be found in [15, 16].

In a different direction, L'Ecuyer, Lécot and Tuffin [50, 51] proposed a randomized quasi-Monte Carlo method, namely the so-called array-RQMC method, which simulates multiple Markov chains in parallel, then applies a suitable permutation to provide a more accurate approximation of the target distribution. It gives an unbiased estimator to the mean and variance and also achieves good empirical performance when randomization is applied to Korobov lattices and Sobol′ point sets.

Gerber and Chopin in [30] adapted low-discrepancy point sets instead of random numbers in the particle filtering framework. They derived a QMC version of particle filtering known as sequential quasi-Monte Carlo (SQMC) methods. They proved consistency and stochastic bounds based on randomized QMC point sets for this algorithm. Numerical evidence confirms that SQMC significantly improves the performance in practice by using Owen scrambled Sobol′ sequences as developed in [66, 67, 68]. The SQMC algorithm developed in this paper can be seen as an extension of array-RQMC to a particle filtering framework. In particular, the essential idea is to generate one QMC point set at each step of the simulation process. Additionally, the convergence results obtained for SQMC also apply to the array-RQMC algorithm proposed in [50] provided the state space is ordered through the Hilbert space-filling curve.

In our work [25], jointly done with Dick and Rudolf, we proved upper bounds on the discrepancy under the assumptions that the Markov chain is uniformly ergodic and the driver sequence is deterministic rather than independent uniformly distributed random variables. In particular, we showed the existence of driver sequences for which the discrepancy of the Markov chain from the target distribution with respect

to certain test sets converges with (almost) the usual Monte Carlo rate of $N^{-1/2}$. In [24], Dick and Rudolf substantially extended the results of [25] to Markov chains which satisfy a much weaker convergence condition. Therein they considered upper bounds on the discrepancy under the assumption that the Markov chain is variance bounding and the driver sequence is deterministic. In particular, they proved a better existence result, showing a discrepancy bound having a rate of convergence of almost N^{-1} under a stronger assumption on the update function, the so-called anywhere-to-anywhere condition. Roughly, variance bounding is a weaker property than geometric ergodicity for reversible chains. It was introduced by Roberts and Rosenthal in [71], who also proved relations among variance bounding, central limit theorems and Peskun ordering, which indicated that variance bounding is a reasonable and convenient property to study for MCMC algorithms.

The copula model is widely used for modelling distributions in financial mathematics by employing the standard uniform univariate margins. The copula-induced discrepancy was introduced by Cambou et al. in [14] and the use of low-discrepancy sequences for copula sampling has been considered. They used randomized low-discrepancy sequences to generate observations from copula models, which yielded good empirical results on financial examples.

The acceptance-rejection algorithm is a widely used technique for sampling from a distribution when direct simulation is not possible or expensive [42]. The basic idea of this method is to find an alternative distribution, often known as proposal distribution, from which we already have an efficient algorithm for generating samples (for instance, the inversion transformation). Then we generate points from the proposal distribution and accept some samples, satisfying a certain condition, as samples of our target distribution. The acceptance-rejection algorithm with deterministic driver sequences is one special class of MCQMC. The deterministic acceptance-rejection algorithm has also been discussed by Moskowitz and Caflisch [56] and Wang [83, 84]. The Halton sequence [33] and Sobol′ sequence [77] were used as the low-discrepancy driver sequences. In [83, 84] a smoothing technique was introduced to improve the numerical performance of the acceptance-rejection

algorithm. Wang [83] gave a heuristic argument to indicate a convergence rate of order $N^{-\frac{s+2}{2(s+1)}}$. This argument assumed that the points in elementary intervals are uniformly distributed. Thus this reasoning is not fully deterministic. The numerical experiments in [83] also indicated an improvement using a well chosen deterministic driver sequence (in this case the so-called Halton sequence [33]) compared to a random driver sequence.

Nguyen and Ökten in [57] presented a consistency result of an acceptance-rejection algorithm for low-discrepancy sequences. This algorithm yielded good numerical performances on standard deviation and efficiency. This algorithm, employing random-start Halton sequences, was used to generate samples from the beta distribution and the gamma distribution, and was also applied in a variance gamma model for option pricing (a generalization of the classical Black-Scholes model for the dynamics of stock prices). However, proving an explicit convergence rate of the discrepancy for this algorithm is still an open problem. See also [56, 57] for numerical experiments using quasi-Monte Carlo point sets for the related problem of integrating indicator functions.

1.3 Our contribution

It is worth noticing that all results regarding deterministic acceptance-rejection samplers given in previous work are empirical evidence and the discrepancy of the generated samples is not directly investigated. Our work focuses on discrepancy properties of points produced by the acceptance-rejection methods, where we consider the construction of driver sequences by digital nets and lattice rules. The combination with the reduced acceptance-rejection sampler for density functions with special structure provides further evidence of the good performance of the deterministic method. We also investigate the discrepancy of samples obtained using the acceptance-rejection algorithm based on stratified inputs. Our algorithm here may also be combined with similar algorithms like the acceptance-complement method. The main contribution in this thesis is the establishment of discrepancy

bounds of samples generated by the acceptance-rejection samplers.

Motivated by previous results, in [92] done with Dick, we consider an acceptance-rejection sampler based on a deterministic driver sequence. The deterministic sequence is chosen such that the discrepancy between the empirical distribution and the target distribution is small. So-called (t, m, s)-nets and (t, s)-sequences constructed based on Sobol′ points are used for this purpose. The empirical evidence shows convergence rates beyond the crude Monte Carlo rate of $N^{-1/2}$. We prove that the discrepancy of samples generated by the QMC acceptance-rejection sampler is bounded from above by $N^{-1/s}$. For a general density, whose domain is the real state space $\mathbb{R}^{s-1}$, the inverse Rosenblatt transformation can be used to convert samples from the $(s-1)$-dimensional cube to $\mathbb{R}^{s-1}$. This way, under certain conditions, the same convergence rate can be achieved for acceptance-rejection samplers on $\mathbb{R}^{s-1}$. In [93], we present an improved convergence rate for a deterministic acceptance-rejection algorithm using $(t, m, s)-$nets as driver sequence. We prove a convergence rate of order $N^{-\alpha}$ for $1/s \leq \alpha < 1$, where α depends on the target density, more explicitly, where the value of α here depends on how well the graph of the target density can be covered by certain rectangles. Some of the results have appeared in the following paper, more details are presented in Chapter 3:

- H. Zhu and J. Dick. Discrepancy bounds for deterministic acceptance-rejection samplers. *Electronic Journal of Statistics*, 8, 678-707, 2014.

In [93] we propose an acceptance-rejection sampler using stratified inputs as driver sequences. We estimate the discrepancy of the N-point set in $(s-1)$-dimensions generated by this algorithm. First we show an upper bound on the star-discrepancy of order $N^{-1/2-1/(2s)}$ for samples generated with respect to the target density. Further we prove an upper bound on the q-th moment of the L_q-discrepancy $(\mathbb{E}[N^q L_{q,N}^q])^{1/q}$ for $2 \leq q \leq \infty$, which is of order $N^{(1-1/s)(1-1/q)}$. Unfortunately, our arguments do not yield an improvement for the case $1 < q < 2$.

From our numerical experiments we can see that, adapting stratified inputs in the acceptance-rejection sampler outperforms the original algorithm. The numerical

results are roughly in agreement with the upper bounds in the theory. The advantage of considering stratified inputs is that it allows us to use probabilistic arguments and consider the average case instead of the worst-case setting. The essential results on this topic are available in the following paper and also Chapter 4 in this thesis.

- H. Zhu and J. Dick. Discrepancy estimations for acceptance-rejection samplers using stratified inputs. *Proceedings of the MCQMC 2014 conference*, Belgium, R. Cools and D. Nuyens (Eds.), Springer, 599-619, 2016.

We prove a lower bound on the star-discrepancy with respect to a concave density function in [92]. The lower bound states that for every driver sequence there is a concave density function such that the convergence rate is at most of order $N^{-2/(s+1)}$ on $[0,1]^{s-1}$, in terms of N points for a density function defined in $[0,1]^{s-1}$. It is natural to ask whether the lower bound is achievable, i.e., can we construct a driver sequence which yields a convergence rate of (almost) $N^{-2/(s+1)}$. To answer this question in dimension one, we propose two types of deterministic constructions in dimension one in [91], where the discrepancy with respect to point sets generated by the deterministic acceptance-rejection sampler is bounded by $N^{-2/3}\log N$ and $N^{-2/3}$ respectively. The construction of driver sequences is explicit and easily implementable, see Chapter 5 for details.

More generally, in [91] we introduce a criterion for measuring the goodness of driver sequences. This criterion has a strong connection with the discrepancy measure. In a nutshell, from the general Erdős-Turán inequality, it can be seen that point sets for which this criterion is small can be used in acceptance-rejection samplers to yield point sets with small discrepancy with respect to the target density measure. A more specific discussion of these results is also available in the following manuscript.

- H. Zhu and J. Dick. A discrepancy bound for deterministic acceptance-rejection samplers beyond $N^{-1/2}$ in dimension 1. *Statistics and Computing*, doi:10.1007/s11222-016-9661-2, 2016.

We also studied the discrepancy in the more general setting for uniformly ergodic Markov chains in [25]. This part is not included in this thesis, for details we refer to our original paper.

- J. Dick, D. Rudolf and H. Zhu. Discrepancy bounds for uniformly ergodic Markov chain quasi-Monte Carlo. *Accepted for publication in The Annals of Applied Probability*, available at arxiv.org/abs/1303.2423, 2016.

The structure of this thesis is as follows. In Chapter 2 we introduce the concept of discrepancy and briefly review the classical low-discrepancy sequences and sampling methods. Chapter 3 gives a detailed discussion of deterministic acceptance-rejection samplers based on digital nets and sequences. In Chapter 4 we consider the acceptance-rejection algorithm with stratified inputs. The explicit constructions achieving a convergence rate beyond $N^{-1/2}$ is presented in Chapter 5. We wrap up this thesis with short concluding remarks and an outlook on future work.

Chapter 2

Preliminaries

2.1 The concept of discrepancy

The concept of discrepancy is introduced to measure the deviation of a sequence from the uniform distribution. For a given point set in the s-dimensional unit cube, the star-discrepancy measures the difference between the proportion of points in a subinterval of $[0,1]^s$ and the Lebesgue measure of this subinterval. Now we give the definition of the so-called local discrepancy which enables us to distinguish the quality of point sets with respect to the uniform distribution, and subsequently we introduce the well-known star-discrepancy and L_q-discrepancy.

Definition 2.1.1. *(local discrepancy). Let $P_N = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N-1}\}$ be a point set in $[0,1)^s$. Define the local discrepancy function as follows:*

$$\Delta_{P_N}(\boldsymbol{t}) = \frac{1}{N}\sum_{n=0}^{N-1} 1_{[\mathbf{0},\boldsymbol{t})}(\boldsymbol{x}_n) - \lambda([\mathbf{0},\boldsymbol{t})), \quad \boldsymbol{t} = (t_1, \ldots, t_s) \in [0,1)^s,$$

where $1_{[\mathbf{0},\boldsymbol{t})}(\boldsymbol{x}_n)$ stands for the indicator function, which is 1 if $\boldsymbol{x}_n$ is in the interval $[\mathbf{0},\boldsymbol{t}) = \prod_{j=1}^{s}[0,t_j)$, and 0 if $\boldsymbol{x}_n \notin [\mathbf{0},\boldsymbol{t})$, and $\lambda(\cdot)$ is the Lebesgue measure.

Figure 2.1 illustrates the local discrepancy of points in a rectangle for a given point set. The local discrepancy of a point set is just the proportion of points in the rectangle $[0,t_1)\times[0,t_2)$ minus the area of the rectangle $[0,t_1)\times[0,t_2)$ (the indicated region in Figure 2.1).

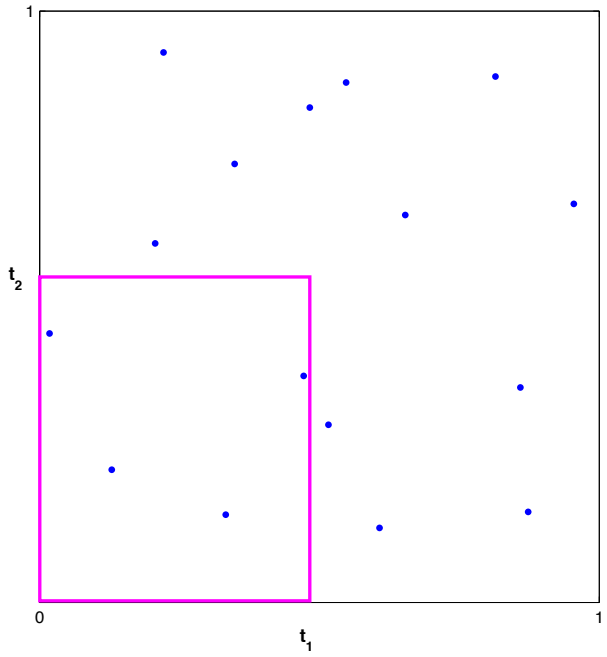


Figure 2.1: Local discrepancy of points in the rectangle $[0, t_1) \times [0, t_2)$. We have $\Delta_{P_N}(t_1, t_2) = 4/16 - t_1 t_2$ in this figure.

The L_q-discrepancy is then the L_q-norm of the local discrepancy function. For $q = \infty$, with the obvious modification of the norm, the L_∞-discrepancy is known as star-discrepancy.

Definition 2.1.2. *(star-discrepancy). Let $P_N = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N-1}\}$ be a point set in $[0, 1)^s$. The star-discrepancy D_N^* is defined by*

$$D_N^*(P_N) = \sup_{\boldsymbol{t} \in [0,1]^s} |\Delta_{P_N}(\boldsymbol{t})|,$$

where the supremum is taken over all $\boldsymbol{t} \in [0, 1]^s$. For an infinite sequence the star-discrepancy is the star-discrepancy of the first N elements of the sequence.

See Figure 2.1 for an illustration of the concept of the star-discrepancy in the unit square. Note that in one-dimension, the star-discrepancy reduces to the Kolmogorov-Smirnov test for the difference between the empirical distribution of the point set $\{x_0, x_1, \ldots, x_{N-1}\}$ and the uniform distribution.

The L_q-discrepancy is defined as the L_q average of the local discrepancy.

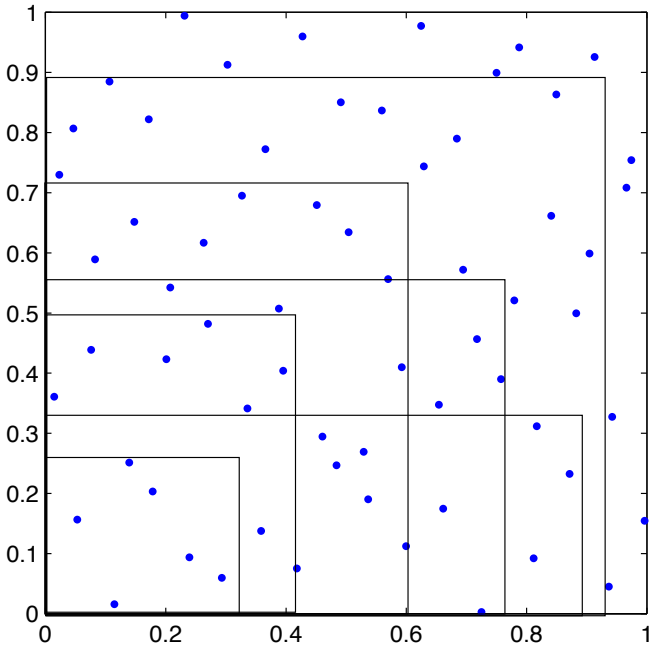


Figure 2.2: The discrepancy measures the difference between the proportion of points in each rectangle J which is anchored at the origin and the Lebesgue measure of J. The star-discrepancy is defined by the supremum of the local discrepancy function over all anchored rectangles J. If we change J to be all rectangles $[\boldsymbol{a}, \boldsymbol{b})$, we obtain the so-called extreme discrepancy.

Definition 2.1.3. *(L_q-discrepancy). Let $P_N = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N-1}\}$ be a point set in $[0,1)^s$. The L_q-discrepancy is defined by*

$$L_q(P_N) = \Big(\int_{[0,1]^s} \big|\Delta_{P_N}(\boldsymbol{t})\big|^q \, \mathrm{d}\boldsymbol{t} \Big)^{1/q}.$$

Very often one uses a slightly stronger version of the star-discrepancy which is commonly known as the extreme discrepancy. Here the definition is extended to all rectangles J of the form $[\boldsymbol{a}, \boldsymbol{b}) = \prod_{j=1}^{s} [a_j, b_j) \subseteq [0,1)^s$ instead of the ones that are anchored at the origin. That is, for a point set $P_N = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N-1}\}$ in $[0,1)^s$, the extreme discrepancy $D_N(P_N)$ of this point set is defined as

$$D_N(P_N) = \sup_{J \subseteq [0,1]^s} \Big| \frac{1}{N} \sum_{n=0}^{N-1} 1_J(\boldsymbol{x}_n) - \lambda(J) \Big|,$$

where J is of the form $[\boldsymbol{a}, \boldsymbol{b}) \subseteq [0,1)^s$.

From these definitions we can conclude a relation between the star-discrepancy and the extreme discrepancy, namely, for any N-element point set P_N in $[0,1)^s$, the following inequalities hold (see [48, Theorem 1.3, pp. 91])

$$D_N^*(P_N) \leq D_N(P_N) \leq 2^s D_N^*(P_N).$$

Note that the discrepancy cannot converge to zero arbitrarily fast, since for any sequence P_N we have

$$\frac{1}{N} \leq D_N(P_N) \leq 1.$$

For a detailed discussion of the extreme discrepancy we refer to, for instance, [48, 60, 23]. We mainly consider the star-discrepancy instead of the extreme discrepancy in the following discussions.

In the estimate of discrepancy, the following triangle inequality for the discrepancy is very useful to obtain an upper bound on the star-discrepancy if the sequence can be decomposed into a number of small point sets.

Proposition 2.1.4. *([48, pp. 115, Theorem 2.6] Triangle inequality for the discrepancy) For $1 \leq i \leq k$, let P_i be point sets in $[0,1]^s$ consisting N_i points with star-discrepancy $D_{N_i}^*(P_i)$. Let P be a superposition of $P_1, \ldots, P_k$ obtained by listing in some order the points of the set P_i, with cardinality $N = N_1 + \ldots + N_k$. Then we have*

$$D_N^*(P) \leq \sum_{i=1}^{k} \frac{N_i}{N} D_{N_i}^*(P_i).$$

The same result holds for the extreme discrepancy with the obvious modification of the notation.

2.2 Construction of low-discrepancy sequences

The discrepancy of certain point sets has been intensively studied and many precise results are known. We now briefly review some explicit construction of point sets which yield small discrepancy. The digital construction of point sets and sequences in quasi-Monte Carlo are well-known.

i	i in base 2	$\phi_2(i)$	decimal form
0	0	0.000	0
1	1	0.100	0.5
2	10	0.010	0.25
3	11	0.110	0.75
4	100	0.001	0.125
5	101	0.101	0.625
6	110	0.011	0.375
7	111	0.111	0.875

Table 2.1: Radical-inverse function in base 2: $\phi_2(i)$ for $i = 0, 1, \ldots, 7$.

The radical-inverse function is commonly used in the construction of low-discrepancy sequences, such as the van der Corput sequence [81] and Halton sequence [33].

Definition 2.2.1. *(radical-inverse function). For integers $i \geq 0$ and $b \geq 2$, the radical-inverse function $\phi_b(i)$ is defined by*

$$\phi_b(i) = \sum_{a=0}^{\infty} \frac{i_a}{b^a},$$

if i has a digital expansion

$$i = \sum_{a=0}^{\infty} i_a b^a,$$

where $i_a \in \mathbb{Z}_b = \{0, 1, \cdots, b-1\}$.

For instance, let $b = 2$, then the corresponding radical inverse function $\phi_2(i)$ and the corresponding decimal form for $i = 0, 1, \ldots 7$ are presented in Table 2.2.

The basic idea of constructing the van der Corput sequence is based on the radical-inverse function.

Definition 2.2.2. *(van der Corput sequence). The van der Corput sequence in base b is the sequence*

$$\phi_b(0), \phi_b(1), \phi_b(2), \cdots .$$

Take $b = 2$ for example. To obtain the corresponding van der Corput sequence, first we write down $0, 1, 2, 3, \cdots$ in base 2, which are

$$0, 1_2, 10_2, 11_2, 100_2, 101_2, 110_2, \ldots,$$

Then by applying the radical-inverse function ϕ_2 to each number we have

$$0, 0.1_2, 0.01_2, 0.11_2, 0.001_2, 0.101_2, 0.011_2, \ldots.$$

In decimal form, it is the sequence

$$0, 0.5, 0.25, 0.75, 0.125, 0.625, 0.375, \ldots.$$

The van der Corput sequence achieves a convergence rate of order $\mathcal{O}(N^{-1} \log N)$ for the star-discrepancy, see [81]. A generalization of the van der Corput sequence to higher dimension is known as Halton sequence from [33], which achieves a star-discrepancy of the first N elements of order $\mathcal{O}(N^{-1}(\log N)^s)$ for an s-dimensional Halton sequence which is constructed as follows.

Definition 2.2.3. *(Halton sequence). Let $p_1, p_2, \cdots, p_s$ be the first s prime numbers. The Halton sequence $\boldsymbol{t}_0, \boldsymbol{t}_1, \boldsymbol{t}_2, \cdots$ in s dimension is given by*

$$\boldsymbol{t}_i = (\phi_{p_1}(i), \phi_{p_2}(i), \cdots, \phi_{p_s}(i)), \qquad i = 0, 1, 2, \ldots.$$

The procedure conducted in the construction of the Halton sequence proceeds as follows. We write down $0, 1, 2, 3, \cdots$ in base $2, 3, 5, \cdots, p_s$ respectively. Then apply the radical-inverse function , which yields the Halton sequence, explicitly given by

$$\begin{aligned}
\boldsymbol{t}_0 &= (0, 0, 0, \cdots, 0), \\
\boldsymbol{t}_1 &= (0, 1_2, 0.1_3, 0.1_5, \cdots, 0.1_{p_s}), \\
\boldsymbol{t}_2 &= (0.01_2, 0.2_3, 0.2_5, \cdots, 0.2_{p_s}), \\
\boldsymbol{t}_3 &= (0.11_2, 0.01_3, 0.3_5, \cdots, 0.3_{p_s}), \\
&\vdots
\end{aligned}$$

Faure and Lemieux in [29] reviewed generalizations of the construction of the original Halton sequence and bounds on the star-discrepancy of these sequences. Another angle to look at the Halton sequence is as follows: The Halton sequence is constructed based on the finer and finer prime-based divisions of sub-intervals of the unit interval in each dimension (i.e. the idea behind the construction of the van der Corput sequence). Then pair them up to obtain a sequence of points in higher dimension.

In [34] Hammersley proposed a construction of an N-element set (known as Hammersley point set) with

$$\boldsymbol{t}_i = \Big(\frac{i}{N}, \phi_{p_1}(i), \phi_{p_2}(i), \cdots, \phi_{p_{s-1}}(i)\Big), \qquad i = 0, 1, 2, \cdots, N-1,$$

where the first component is evenly spaced and the remaining positions are filled by components as in the Halton sequence. The star-discrepancy is improved, there is one power less of $\log N$ compared with that of the Halton sequence, that is, it converges with $\mathcal{O}(N^{-1}(\log N)^{s-1})$.

The Hammersley point set and Halton sequence represent two types of quasi-Monte Carlo methods, which are the closed type and the open one. The closed type methods use a finite point set, the construction depends on the number of points N. Changing the number of points means that the point set will be changed. On the contrary, the open type points are extensible in the number of sample points without discarding the samples already used. In other words, increasing N will not change the first N points for the open type construction, since it just take additional points from an infinite sequence with the first N points remaining the same. Regarding the comparison between the closed type and open type constructions and their impact on the convergence analysis will be further discussed in Chapter 5.

The area of quasi-Monte Carlo methods has been enriched with the development of digital nets and sequences as well as the theory of lattice rules. Explicit constructions of (t, s)-sequences in base 2 have been found by Sobol′ [77], in prime base $b \geq s$ by Faure [28] and in prime-power base b by Niederreiter [59]. We here present the explicit construction based on Sobol′ sequences only. More general prop-

erties of digital nets are presented in Chapter 3.

Definition 2.2.4. *(Sobol′ sequences). To generate the j-th component of the points in a Sobol′ sequences, let p_j be primitive polynomial over the finite field $\mathbb{Z}_2$ for $j = 1, 2, \cdots, s$, of degree e_j given by*

$$p_j(x) = x^{e_j} + a_{1,j}x^{e_j-1} + a_{2,j}x^{e_j-2} + \ldots + a_{e_j-1,j}x + 1,$$

where the coefficients $a_{1,j}, a_{2,j}, \ldots, a_{e_j-1,j} \in \mathbb{Z}_2$.

Define a sequence of positive odd numbers $\{m_{1,j}, m_{2,j}, \ldots m_{e_j,j}\}$ such that $m_{k,j} < 2^k$ for $1 \leq k \leq e_j$, where $m_{k,j}$ is defined by the recurrence formula

$$m_{k,j} = 2a_{1,j}m_{k-1,j} \oplus 2^2 2_{2,j}m_{k-2,j} \oplus \ldots \oplus 2^{e_j-1}a_{e_j-1}m_{k-e_j+1,j} \oplus 2^{e_j}m_{k-e_j,j} \oplus m_{k-e_j,j},$$

where $\oplus$ is the bit-by-bit operator. The so-called direction numbers $\{v_{1,j}, v_{2,j}, \ldots\}$ are defined by

$$v_{k,j} = \frac{m_{k,j}}{2^k}, \qquad \text{for } k \geq 1.$$

Then $x_{i,j}$, the j-th component of the i-th point in a Sobol′ sequence, is given by

$$x_{i,j} = i_0 v_{1,j} \oplus i_1 v_{2,j} \oplus \ldots \oplus i_{r-1} v_{r,j},$$

for $i \in \mathbb{N}_0$ with the dyadic expansion $i = i_0 + 2i_1 + \ldots + 2^{r-1}i_{r-1}$.

Antonov and Saleev in [5] proposed a more efficient Gray code implementation of the Sobol′ sequence. Joe and Kuo in [43] have optimized the choice of the so-called direction numbers $m_{k,j}$ of Sobol′ sequences using two-dimensional projections as quality criterion.

Lattice rules provide a different mechanism for the construction of low-discrepancy point sets. The simplest example is a rank one lattice. An N-element rank-1 lattice is a quasi-Monte Carlo method with quadrature points

$$\boldsymbol{t}_j = \left\{\frac{j\boldsymbol{z}}{N}\right\}, \qquad j = 0, 1, 2, \ldots, N-1,$$

where $\boldsymbol{z}$ is the generating vector having no factor in common with N, and the bracket $\{\,\}$ means to take the fractional part $\{x\} = x - \lfloor x \rfloor, x \in \mathbb{R}, x \geq 0$, of all components.

A good rank-1 lattice relies on the construction of a good generating vector. The component-by-component algorithm proposed independently by [45, 46] by Sloan and Reztsov [76] addresses this problem. The component-by-component algorithm constructs the generating vector one component at a time, in each step minimizing a certain error measure for the cubature rule and keeping all previously chosen components fixed.

Let $\boldsymbol{z} = (z_1, z_2, \ldots, z_s)$ be the generating vector, the generic component-by-component algorithm works in the following way to determine $\boldsymbol{z}$:

- Set $z_1 = 1$.
- For $k = 2, \ldots, s$, assume that we have found $z_2, \ldots, z_{k-1}$. Then we search for z_k by minimizing the error criterion (for example, the worst-case error defined in Equation 2.3.1 below) as a function of z_k.

Convergence analysis for the component-by-component construction has been done. Korobov in [46, Theorem 18, pp. 120] proved the optimal convergence rate of periodic function space. Kuo in [49] showed that those lattice rules constructed by the component-by-component algorithm actually achieve the optimal rate of convergence under appropriate conditions on the weights in weighted Korobov and Sobolev spaces. Further improvement and convergence analysis has been made by Dick [20] and Dick and Kuo in [19]. Furthermore the fast component-by-component construction due to Nuyens and Cools [63] uses the fast Fourier transform.

If one chooses a generating vector $\boldsymbol{z} = (1, F_k)$ and $N = F_{k+1}$ with F_k the k-th Fibonacci number, the corresponding lattice rule is known as a Fibonacci rule. We will discuss the discrepancy properties of Fibonacci rules in more detail in Chapter 5. A summary of lattice methods can be found in the monograph [75], more recent development of lattice rules is reviewed in [22, Section 5].

Randomization of quasi-Monte Carlo point sets has also drawn a significant amount of attention in this area. The idea is to introduce a random element into the deterministic construction of the point set, which allows us to view them as variance reduction techniques. There are a couple of benefits of randomization. Firstly it

yields an unbiased estimator. Secondly, since there is a statistical error estimate, one can use probabilistic arguments to analyse the errors involved in quasi-Monte Carlo methods. Most importantly, the randomization preserve the good discrepancy properties of the point set. Recent development of randomization of quasi-Monte Carlo and application to many different problems are summarized in [52, 53].

Various randomization are known, the main randomization techniques used on quasi-Monte Carlo methods include shifting and scrambling. For instance, we can introduce a shift in lattice rules by choosing $\Delta \in [0,1]^s$ uniformly distributed. The shifted lattice rule is given by

$$\boldsymbol{t}_j = \left\{ \frac{j\boldsymbol{z}}{N} + \Delta \right\}, \qquad j = 0, 1, 2, \ldots, N-1.$$

Shifting can be done to sequences other than lattice point sets, randomly shifted Halton sequences have been considered by Wang and Hickernell [82].

Scrambled sequences have been introduced by Owen in [66, 67, 68]. The idea is to scramble the digits of special low-discrepancy sequences, the (t, s)-sequences in base b by using random permutations of the digits so that the good discrepancy properties of the original point set are retained. Further analysis of scrambling algorithms are presented in [69, 87, 88], for details, we refer to the original papers.

Stratification is an efficient variance reduction technique. It has a wide practical utility due to a simple implementation [31, Chapter 4] and [55]. For the simplest case where the integration domain $D = [0,1]$, the stratification technique first splits $[0,1]$ to M subsets with equal length $1/M$, i.e.

$$[0,1] = \bigcup_{i=0}^{M-1} \left[\frac{i}{M}, \frac{i+1}{M} \right],$$

then computes the integral in $[0,1]$ as follows

$$\int_{[0,1]} f(x)\,\mathrm{d}x = \sum_{i=0}^{M-1} \int_{i/M}^{(i+1)/M} f(x)\,\mathrm{d}x.$$

Each integral in the subset $[i/M, (i+1)/M]$ is then approximated by the same number of quadrature points uniformly distributed in $[i/M, (i+1)/M]$ for $i = 0, \ldots, M-1$.

For the integration domain $D = [0,1]^s$, the grid-based stratified sampling is conducted in the following way: Let

$$[0,1]^s = \bigcup_{i=0}^{M-1} Q_i,$$

where each Q_i is of volume $1/M$. In order to construct a well distributed point set in $[0,1]^s$, it is reasonable to have the same number of points in each subset Q_i. Stratified technique can also go beyond the equal-volume splitting, then the number of points in each strata is determined according to the measure proportion of the strata.

The efficiency of stratified inputs for variance reduction has been studied in [55, Section 4.4]. Compared with classical methods, stratification sampling has the advantage to give an unbiased estimate along with the variance reduction. More precisely, grid-based stratified sampling improves the root mean square error to $N^{-1/2-1/s}$ for Monte Carlo. Combined with antithetic sampling it can further reduce the variance. More generalized stratification technique include Latin hypercube sampling and orthogonal array sampling, see for instance [65, Chapter 10]. For other variance reduction techniques can refer to Lemieux [53, Chapter 4] where the most commonly used techniques are reviewed. In Chapter 4 of this thesis, we will employ stratified inputs for the acceptance-rejection algorithm to obtain good samples for non-uniform target distributions.

Low-discrepancy point sets and sequences have also been considered for domains other than intervals. For instance, the discrepancy in terms of the family of convex sets is known as isotropic discrepancy introduced by Zaremba [89]. Schmidt in [74] studied the irregularities of distribution for the special classes of convex sets such as rectangles, balls and spherical caps.

The definition of discrepancy can also be extended to non-uniform distributions, we defer the relevant discussion to the following chapters of this thesis. We will use the acceptance-rejection technique to explicitly construct point sets for non-uniform measures in Chapter 3–5, then analyse the discrepancy properties of the corresponding samples.

2.3 Numerical integration and the Koksma-Hlawka inequality

One important application of discrepancy is in numerical integration. Suppose we approximate the s-dimensional integrand $\int_{[0,1]^s} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$ by the equal weight quadrature rule

$$\int_{[0,1]^s} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \approx \frac{1}{N}\sum_{n=0}^{N-1} f(\boldsymbol{x}_n),$$

where $\{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N-1}\}$ is an N-element point set in $[0,1]^s$. To measure the quality of the approximation, the Koksma–Hlawka inequality provides a tight error bound on the approximation error of an integral by the sample average of integrand values at some quadrature points.

Proposition 2.3.1. *(Koksma-Hlawka inequality). Let f be a measurable function on $[0,1]^s$ which has bounded variation $V_p(f) < \infty$. Let $P_N = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N-1}\}$ be a point set in $[0,1]^s$. Then*

$$\left| \int_{[0,1]^s} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} - \frac{1}{N}\sum_{n=0}^{N-1} f(\boldsymbol{x}_n) \right| \leq V_p(f) L_q(P_N),$$

where $1/p + 1/q = 1$, $p, q \geq 1$, and $V_p(f)$ denotes the variation of f in the sense of Hardy-Krause.

Note that there are different ways to define the variation, we follow the definition in the sense of Hardy-Krause presented in Section 5.2.3 of this thesis. See also [60, Chapter 2] and [21, Section 3.1].

For the simplest one-dimensional case, a special case of this inequality can be deduced as follows. Let

$$f(x) = f(1) - \int_0^1 f'(t) 1_{[x,1)}(t)\,\mathrm{d}t,$$

then

$$\int_0^1 f(x)\,\mathrm{d}x - \frac{1}{N}\sum_{n=0}^{N-1} f(x_n) = \int_0^1 f'(t) \left[\frac{1}{N}\sum_{n=0}^{N-1} 1_{[x_n,1]}(t) - \int_0^1 1_{[x,1]}(t)\,\mathrm{d}x \right] \mathrm{d}t.$$

Now use Hölder's inequality,

$$\left| \int_0^1 f(x)\,\mathrm{d}x - \frac{1}{N}\sum_{n=0}^{N-1} f(x_n) \right| \leq \left(\int_0^1 |f'(t)|^p\,\mathrm{d}t \right)^{1/p} \quad L_q(P_N),$$

to obtain a version of the Koksma-Hlawka inequality, where $L_q(P_N)$ is the discrepancy of quadrature points, and the remaining part is the corresponding definition of variation of the integrand in dimension one.

The classical Koksma-Hlawka inequality was first proved by Koksma [44] for dimension $s = 1$. Hlawka [41] extended the result to arbitrary dimension $s \geq 1$. This inequality has been developed for a larger function class where the integrand is piecewise smooth in [12]. Note that currently the inequality in Proposition 2.3 is based on uniform distribution. This has been generalised to a non-uniform distribution by Aistleitner and Dick in [2]. We defer the discussion of this case to Chapter 5. More variations of the Koksma-Hlawka type inequality are summarized in [35]. For domains other than cubes, Zaremba [89] proved a similar Koksma-Hlawka type inequality for a convex integration domain in terms of the isotropic discrepancy.

The integration error depends on two quantities, namely, the quadrature points and the integrand function. For a fixed integrand function class, the integration error depends on the discrepancy properties of the quadrature points. That is part of our motivation to move from Monte Carlo method to quasi-Monte Carlo method to obtain better quadrature points and hence reduce the integration error.

Another useful principle used to measure the efficiency of numerical integration algorithms is the worst-case integration error which is defined by the worst-case performance of integration over the unit ball of functions in some function class. Let f belong to some function class $\mathcal{H}$ with norm $\|\cdot\|$. The worst-case error is denoted by

$$e(\mathcal{H}, P_N) = \inf_{\|f\|\leq 1, f\in\mathcal{H}} \left| \int_{[0,1]^s} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} - \frac{1}{N}\sum_{n=0}^{N-1} f(\boldsymbol{x}_n) \right|. \tag{2.3.1}$$

If $\mathcal{H}$ is a reproducing kernel Hilbert space with reproducing kernel $K(\boldsymbol{x}, \boldsymbol{y})$, we have an exact formula for the squared worst-case error given as

$$e^2(\mathcal{H}, P_N) = \int_{[0,1]^{2s}} K(\boldsymbol{x}, \boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - \frac{2}{N}\sum_{n=0}^{N-1}\int_{[0,1]^s} K(\boldsymbol{x}_n, \boldsymbol{y})\,\mathrm{d}\boldsymbol{y} + \frac{1}{N^2}\sum_{m,n=0}^{N-1} K(\boldsymbol{x}_n, \boldsymbol{x}_m). \tag{2.3.2}$$

For investigating the numerical integration error in a reproducing kernel Hilbert space $\mathcal{H}$, we only need to know the reproducing kernel for the function space $\mathcal{H}$, then we can derive the worst-case error. For equal weight cubature rules, the worst-case error is just another kind of discrepancy.

With a special choice of reproducing kernel, one can derive an explicit formula for the L_2-discrepancy, see Proposition 4.1.2 or [23, Proposition 2.15] and the relevant discussion therein.

2.4 Quick review of sampling methods

Sampling from a known or partially known distribution arises in many fields of simulation, ranging from computer science, engineering and finance, to Bayesian statistics. In this section, we present a quick review of sampling methods which are of great interest to us. Regarding a complete discussion of Monte Carlo and quasi-Monte Carlo sampling together with implementation and application to finance, see [53]. For more details on non-uniform random variate generation we also refer to the monographs [18, 42].

Let F be a continuous distribution function on R and let the inverse function F^{-1} be defined by $F^{-1}(u) = \inf\{x : F(x) \geq u, u \in [0,1]\}$. If u is uniformly distributed in $[0,1]$, i.e. $u \sim U([0,1])$, then $F^{-1}(u)$ has distribution F. Moreover, if X has distribution F, $F(X)$ consequently is uniformly distributed. Thus, based on this property, in order to generate a random variable X according to the cumulative distribution function F, it suffices to generate a uniform random variable in $[0,1]$, then apply the inverse transformation such that $x = F^{-1}(u)$ to get the correct distribution. Note that the inverse transformation can be used to generate random variables with distribution F provided that F^{-1} is explicitly known. In the

framework of quasi-Monte Carlo methods, the inversion transform is also the first choice when it is available due to the measure preserving property. We will explore more in this direction in Chapter 3. Unfortunately many distributions do not have a closed form CDF and computing the inverse CDF is often comparatively expensive, for distributions such as normal, gamma and beta-distributions.

Besides the inversion principle, some transformations have been proposed for sampling from certain distributions by using special properties of the distribution. For instance, Box and Müller in [10] proposed a reliable and speedy method known as Box-Müller transform to generate the bivariate Gaussian by realising that the bivariate Gaussian variate are just two independent standard normal variates.

Let u_1, u_2 be uniformly distributed in $[0, 1]$. The following transformation yields that (X_1, X_2) has the standard normal distribution $\mathcal{N}(0, 1)$,

$$\begin{aligned} X_1 &= \sqrt{-2\log u_1}\cos(2\pi u_2), \\ X_2 &= \sqrt{-2\log u_1}\sin(2\pi u_2). \end{aligned}$$

Furthermore, with an obvious modification of the transform, it can be used to generate a variable $(Z_1, Z_2) \sim \mathcal{N}(\mu, \sigma)$ via

$$\begin{aligned} Z_1 &= \mu + \sigma\sqrt{-2\log u_1}\cos(2\pi u_2), \\ Z_2 &= \mu + \sigma\sqrt{-2\log u_1}\sin(2\pi u_2). \end{aligned}$$

A quasi-Monte Carlo version of Box-Müller is considered by Ökten and Göncü in [64]. They concluded that the Box-Müller method is a good alternative to the inverse transformation method for generating low-discrepancy sequences from the normal distribution. For functions having certain further properties, theoretical along with numerical evidence suggests that Box-Müller outperforms the inversion method.

Unfortunately, this type of construction greatly depends on special properties of the distribution, which are not applicable to large families of distributions. Now we present a more universal sampling method, the so-called acceptance-rejection algorithm. The basic idea of this algorithm is first to find a distribution from which there is an efficient way to sample, then apply the acceptance-rejection procedure to obtain samples from the target distribution.

We present the acceptance-rejection algorithm in more detail. Let $\psi : D \to \mathbb{R}_+$ be our target density function, where $D \subseteq \mathbb{R}^{s-1}$ and $\mathbb{R}_+ = [0, \infty)$. Assume that it is not possible or expensive to sample directly from the target distribution. The following algorithm can be used to obtain samples with respect to the target distribution ψ by choosing a proposal density H from which we can sample.

Algorithm 2.4.1. *(Acceptance-rejection algorithm based on random inputs). Given a target density $\psi : D \to \mathbb{R}_+$ and a proposal density $H : D \to \mathbb{R}_+$. Assume that there exists a constant $L < \infty$ such that $\psi(\boldsymbol{x}) < LH(\boldsymbol{x})$ for all $\boldsymbol{x}$ in the domain D. We introduce another random variable u having uniform distribution in the unit interval, i.e. $u \sim U([0,1])$. Then the acceptance-rejection algorithm is given by*

1. *Draw $X \sim H$ and $u \sim U([0,1])$.*
2. *Accept $Y = X$ as a sample of ψ if $u \leq \frac{\psi(\boldsymbol{X})}{LH(\boldsymbol{X})}$, otherwise go back to step 1.*

The following argument verifies the validity of the acceptance-rejection method. Let the accepted sample set $Y = \{\text{X accepted}\}$. We just need to show that the conditional distribution of Y given that $u \leq \frac{\psi(Y)}{LH(Y)}$ is indeed the distribution with respect to ψ, that is

$$\mathbb{P}\left(Y \leq \boldsymbol{y} \mid u \leq \frac{\psi(Y)}{LH(Y)}\right) = \int_{(-\infty, \boldsymbol{y}]} \psi(\boldsymbol{z})\, \mathrm{d}\boldsymbol{z},$$

where $(-\infty, \boldsymbol{y}] = \prod_{j=1}^{s-1}(-\infty, y_j)$ and $Y \leq \boldsymbol{y}$ means that $Y_j \leq y_j$ for $j = 1, \ldots, s-1$ with $Y = (Y_1, \ldots Y_{s-1})$. This equation holds since

$$\begin{aligned}
\mathbb{P}\left(Y \leq \boldsymbol{y} \mid u \leq \frac{\psi(Y)}{LH(Y)}\right) &= \frac{\mathbb{P}\left(Y \leq y, u \leq \frac{\psi(Y)}{LH(Y)}\right)}{\mathbb{P}\left(u \leq \frac{\psi(Y)}{LH(Y)}\right)} \\
&= \frac{1}{\mathbb{P}\left(u \leq \frac{\psi(Y)}{LH(Y)}\right)} \int_{(-\infty, \boldsymbol{y}]} \int_{\left[0, \frac{\psi(\boldsymbol{z})}{LH(\boldsymbol{z})}\right]} H(\boldsymbol{z})\, \mathrm{d}u\, \mathrm{d}\boldsymbol{z} \\
&= \frac{1}{\mathbb{P}\left(u \leq \frac{\psi(Y)}{LH(Y)}\right)} \int_{(-\infty, \boldsymbol{y}]} \frac{\psi(\boldsymbol{z})}{LH(\boldsymbol{z})} H(\boldsymbol{z})\, \mathrm{d}\boldsymbol{z} \\
&= \frac{1}{\mathbb{P}\left(u \leq \frac{\psi(Y)}{LH(Y)}\right)} \int_{(-\infty, \boldsymbol{y}]} \frac{\psi(\boldsymbol{z})}{L}\, \mathrm{d}\boldsymbol{z},
\end{aligned}$$

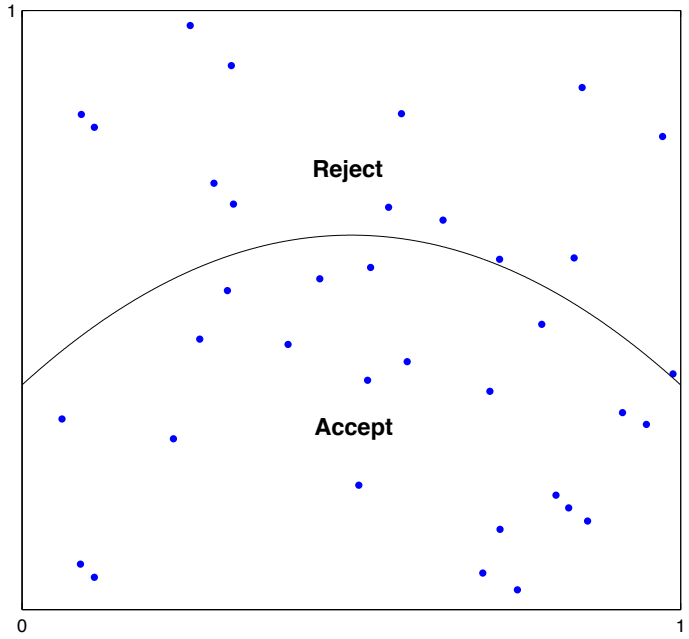


Figure 2.3: Acceptance-rejection sampler with the proposal density $H(x) = 1$.

and by realising $\mathbb{P}\left(u \leq \frac{\psi(Y)}{LH(Y)}\right) = 1/L$, we get the desired result.

The acceptance-rejection sampler works to sample from an unknown density based on a proposal density (or hat function) through a rather simple procedure. The toy problem in Figure 2.3 illustrates the basic idea of this algorithm where we choose the uniform distribution as the proposal density, and hence propose points randomly in the unit square. This algorithm works by only accepting points lying under the target density curve. Once we project all accepted points onto the first coordinate, these points in the interval $[0, 1]$ have the desired distribution as the indicated graph in the figure.

A way to optimize acceptance-rejection algorithms is by designing good proposal densities. One can choose a proposal density from a large family by determining the value of parameters to control the acceptance rate and the constant L involved in the algorithm. For a log-concave density, a generic adaptive acceptance-

rejection method is quite efficient, however it is beyond our interests for the discussion of designing proposal densities. See [9], [18, Chapter 2] and [42, Chapter 4&5] the references therein on this topic. We are more interested on the properties of samples obtained from an acceptance-rejection sampler with respect to the discrepancy measure based on a simple choice of proposal density. This leads us to consider the role of samples having the proposal density (we call it driver sequence throughout the thesis).

Let us revisit the toy problem illustrated in Figure 2.3 for a density defined in $[0, 1]$. Figure 2.4 shows a comparison between different driver sequences for this example: deterministic points (Sobol′ points) and pseudo-random points. The total number of points in each case is 2^9 and the histograms are with respect to samples we accepted. The acceptance-rejection sampler works by only accepting those points under the target density curve. The difference of driver sequences obviously affects the samples we obtain by the acceptance-rejection algorithm, hence the distribution properties of the points which were accepted will be influenced. The right two figures in Figure 2.4 show the histograms of the points which we accepted in both cases. Note that the number of accepted samples is roughly equal but the deterministic samples better estimate the density function. Additionally, from the superior distribution properties in terms of the discrepancy of the Sobol′ sequence, one could expect an improvement in the discrepancy of the samples obtained from the acceptance-rejection algorithm based on the Sobol′ sequence.

Acceptance-rejection sampling and importance sampling [70, Section 3] are quite similar ideas. Both of them distort samples from a proposal distribution in order to sample from another one. However, there is a difference in the selection of the constant $L > \psi(\boldsymbol{x})/H(\boldsymbol{x})$ for $\boldsymbol{x}$ in the domain D. The acceptance-rejection method does not work when $\sup_{\boldsymbol{x}\in D} \psi(\boldsymbol{x})/H(\boldsymbol{x}) = \infty$, while importance sampling is still available [65]. In this thesis, we only use the acceptance-rejection sampler to get samples of a given target density, since we are interested in obtaining discrepancy bounds for non-uniform distributions. The role of importance sampling in quasi-Monte Carlo methods is left to future work.

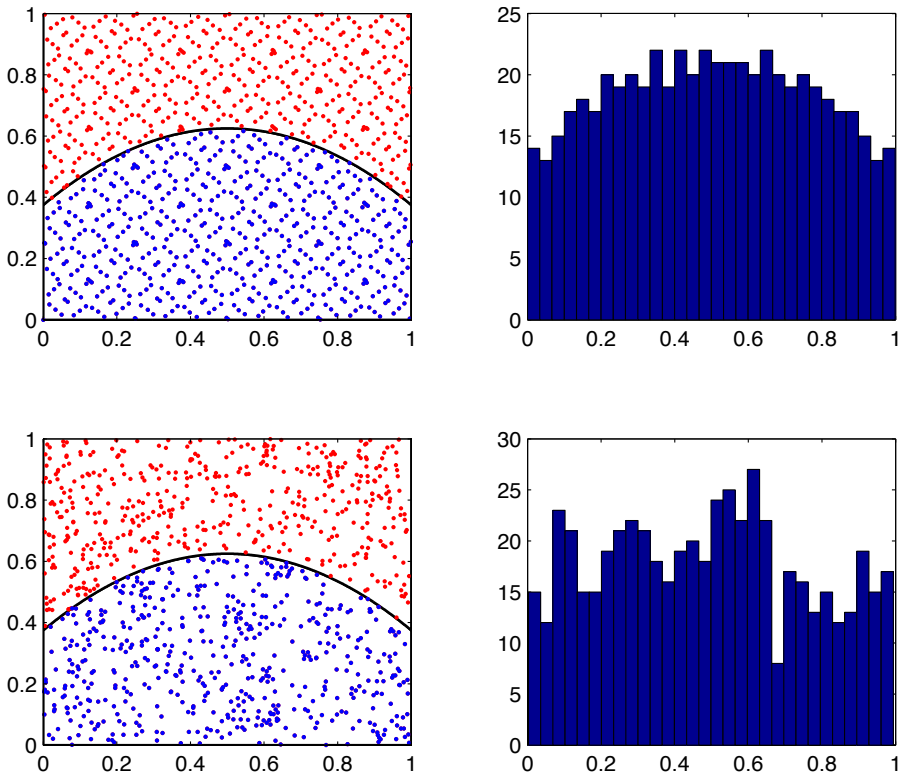


Figure 2.4: Different driver sequences: deterministic and pseudo-random points.

More generally, Markov chains can be used to generate samples whose stationary distribution approximates a given target distribution. The Metropolis-Hastings algorithm, Slice sampler and Gibbs sampler are of great interest in this area. The corresponding quasi-Monte Carlo versions of those sampling methods have been considered by Tribble [79] and Chen [15] by using completely uniformly distributed sequences instead of pseudo-random sequences. An explicit construction of driver sequences for these samplers which yield the optimal order of convergence is not yet available.

Chapter 3

Discrepancy bounds for the acceptance-rejection sampler using (t, m, s)-nets

3.1 Background

In this chapter we consider the deterministic acceptance-rejection sampler based on digital nets. We first establish some notation and some useful definitions and then obtain preliminary theoretical results in Section 3.1. Section 3.2 presents an upper bound and a lower bound for the star-discrepancy of samples generated with respect to a target density function defined in the unit cube $[0,1]^{s-1}$ and real state space $\mathbb{R}^{s-1}$ respectively. An improved upper bound is also proved in this section for target density functions with certain properties. Section 3.3 contains the discussion of a quasi-Monte Carlo version of the reduced acceptance-rejection sampler. Using the δ-cover technique presented in Section 3.4, numerical experiments in Section 3.5 verify the efficiency of the deterministic acceptance-rejection algorithms.

Now we first introduce the definition of (t, m, s)-nets and (t, s)-sequence which we use as the driver sequence throughout this chapter. The following fundamental definitions of elementary interval and fair sets are used to define a (t, m, s)-net and

(t, s)-sequence in base b.

Definition 3.1.1. *(b-adic elementary interval). Let $b \geq 2$ be an integer. An s-dimensional b-adic elementary interval is an interval of the form*

$$\prod_{i=1}^{s} \left[\frac{a_i}{b^{d_i}}, \frac{a_i + 1}{b^{d_i}} \right),$$

with integers $0 \leq a_i < b^{d_i}$ and $d_i \geq 0$ for all $1 \leq i \leq s$. If $d_1, \ldots, d_s$ are such that $d_1 + \cdots + d_s = k$, then we say that the elementary interval is of order k.

Definition 3.1.2. *(fair sets). For a given set $P_N = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N-1}\}$ consisting of N points in $[0, 1)^s$, we say for a subset J of $[0, 1)^s$ to be fair with respect to P_N, if*

$$\frac{1}{N} \sum_{n=0}^{N-1} 1_J(\boldsymbol{x}_n) = \lambda(J),$$

where $1_J(\boldsymbol{x}_n)$ is the indicator function of the set J and λ is the Lebesgue measure. The notation can also be used the other way around, namely, we can also say P_N is fair with respect to a subset J if the above equation holds.

Definition 3.1.3. *((t, m, s)-nets in base b). For a given dimension $s \geq 1$, an integer base $b \geq 2$, a positive integer m and an integer t with $0 \leq t \leq m$, a point set $Q_{m,s}$ of b^m points in $[0, 1)^s$ is called a (t, m, s)-net in base b if the point set $Q_{m,s}$ is fair with respect to all b-adic s-dimensional elementary intervals of order at most $m - t$.*

Definition 3.1.4. *((t, s)-sequence). For a given dimension $s \geq 1$, an integer base $b \geq 2$ and a positive integer t, a sequence $\{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots\}$ of points in $[0, 1)^s$ is called a (t, s)-sequence in base b if for all integers $m \geq t$ and $k \geq 0$, the point set consisting of the points $\boldsymbol{x}_{kb^m}, \ldots, \boldsymbol{x}_{kb^m + b^m - 1}$ forms a (t, m, s)-net in base b.*

To provide an intuitive understanding of the idea of digital nets, Figures 3.1 to 3.3 show the essential property of (t, m, s)-nets in base b. For simplicity, we demonstrate digital nets in base 2 in two dimension.

For a two-point set to form a $(0, 1, 2)$-net in base 2 means that every elementary interval (there are two types of elementary interval in this case) of volume one half

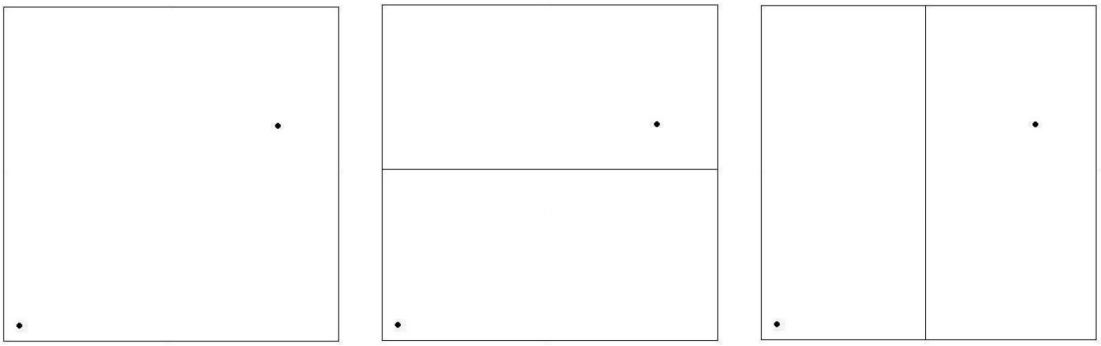


Figure 3.1: $(0, 1, 2)$-nets in base 2.

contains exactly $2^0 = 1$ point of the given point set. The property remains if we increase the number of points and reduce the size of the elementary interval accordingly. For instance, a 4-point set forms a $(0, 2, 2)$-net in base 2 means that every elementary interval (there are three types of elementary intervals) of volume one quarter contains exactly 1 point of the point set. See Figures 3.1 to 3.3 for the elementary intervals for $(0, 1, 2)$-net, $(0, 2, 2)$-net and $(0, 3, 2)$-net in base 2 respectively.

Explicit constructions of (t, s)-sequences in base 2 have been found by Sobol′ [77], in prime base $b \geq s$ by Faure [28] and in prime-power base b by Niederreiter [59]. In all these constructions t depends only on s but not on m. The construction based on Sobol′ is presented in Section 2.1. In practice, since the construction of digital nets are included in the statistics toolbox of Matlab, this method is very easy to implement. Readers seeking more discussion of construction methods can also consult [23, Chapters 4&8].

Now we recall the definition of the star-discrepancy which enables us to distinguish the quality of point sets with respect to the uniform distribution. The star-discrepancy D_N^* with respect to a point set $P_N = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N-1}\}$ in the s-dimensional cube is defined by

$$D_N^*(P_N) = \sup_{J \subset [0,1)^s} \left| \frac{1}{N} \sum_{n=0}^{N-1} 1_J(\boldsymbol{x}_n) - \lambda(J) \right|,$$

where the supremum is taken over all $J = \prod_{i=1}^{s} [0, \beta_i) \subseteq [0, 1)^s$.

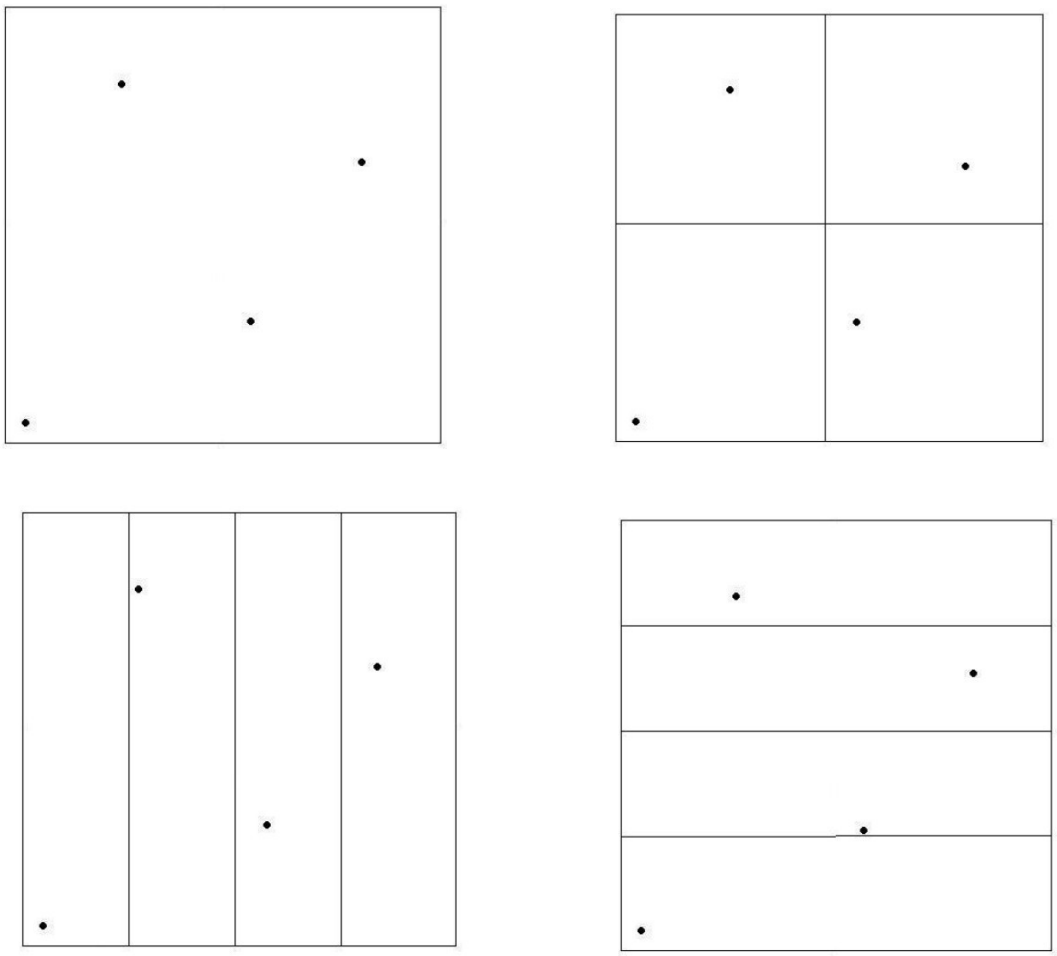


Figure 3.2: $(0, 2, 2)$-nets in base 2.

We need various other types of discrepancies for our analysis. If we extend the supremum in the star-discrepancy to all convex sets in $[0, 1]^s$, we get another interesting discrepancy introduced by Zaremba [89], the so-called isotropic discrepancy. It is a measure of the distribution properties of point sets with respect to convex sets. This quantity is instrumental for establishing effective error bounds in quasi-Monte Carlo integration over bounded convex sets, see [90].

Definition 3.1.5. *(isotropic discrepancy). Let $P_N = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N-1}\}$ be a point set in $[0, 1)^s$. The isotropic discrepancy J_N is defined to be*

$$J_N(P_N) = \sup_{J \subseteq \mathcal{C}} \left| \frac{1}{N} \sum_{n=0}^{N-1} 1_J(\boldsymbol{x}_n) - \lambda(J) \right|,$$

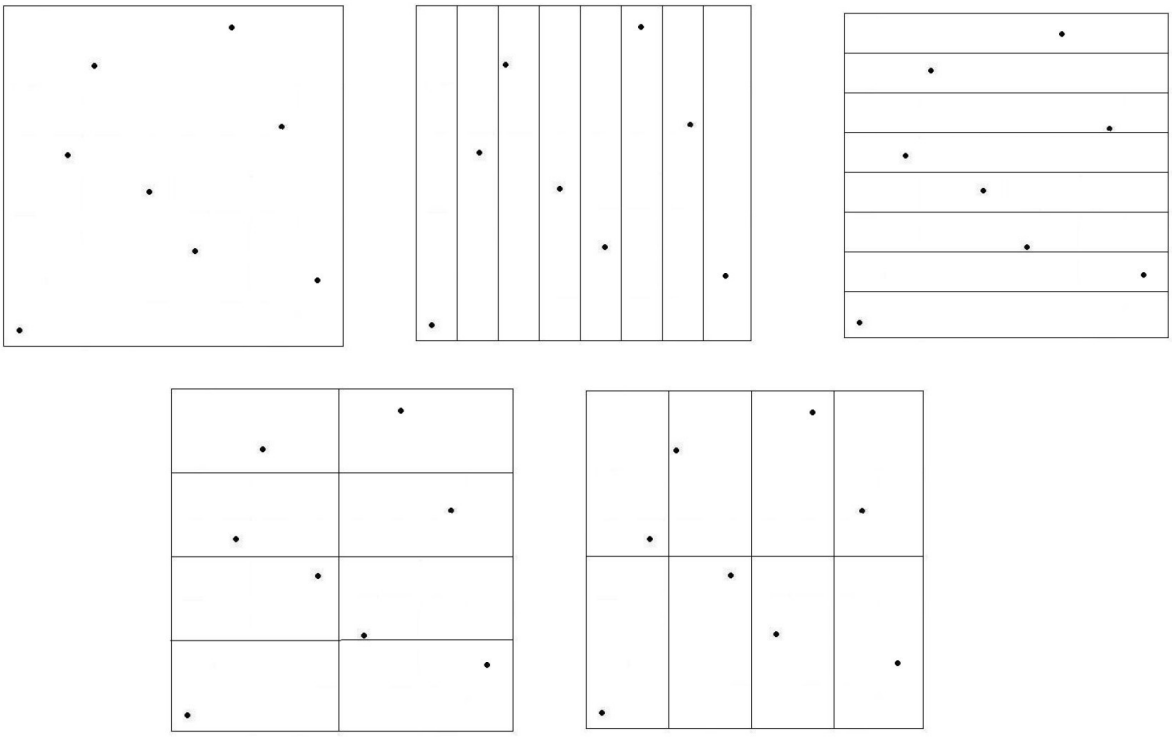


Figure 3.3: $(0, 3, 2)$-nets in base 2.

where $\mathcal{C}$ is the family of all convex subsets of $[0, 1)^s$.

The connection between isotropic discrepancy and extreme discrepancy is established in [61] by Niederreiter and Wills. For any point set $P_N \subseteq [0, 1]^s$, we always have

$$D_N(P_N) \leq J_N(P_N) \leq 4sD_N(P_N)^{1/s}.$$

For further reading about the definition and properties of isotropic discrepancy, we refer for instance to [48, 60].

For our purposes here we need the definition of pseudo-convex sets which we introduce in the following (see also [1, Definition 2]).

Definition 3.1.6. *(pseudo-convex set). Let A be an open subset of $[0, 1]^s$ such that there exists a collection of p convex subsets $A_1, \ldots, A_p$ of $[0, 1]^s$ satisfying*

1. *$A_i \cap A_j = \emptyset$ for $i \neq j$,*

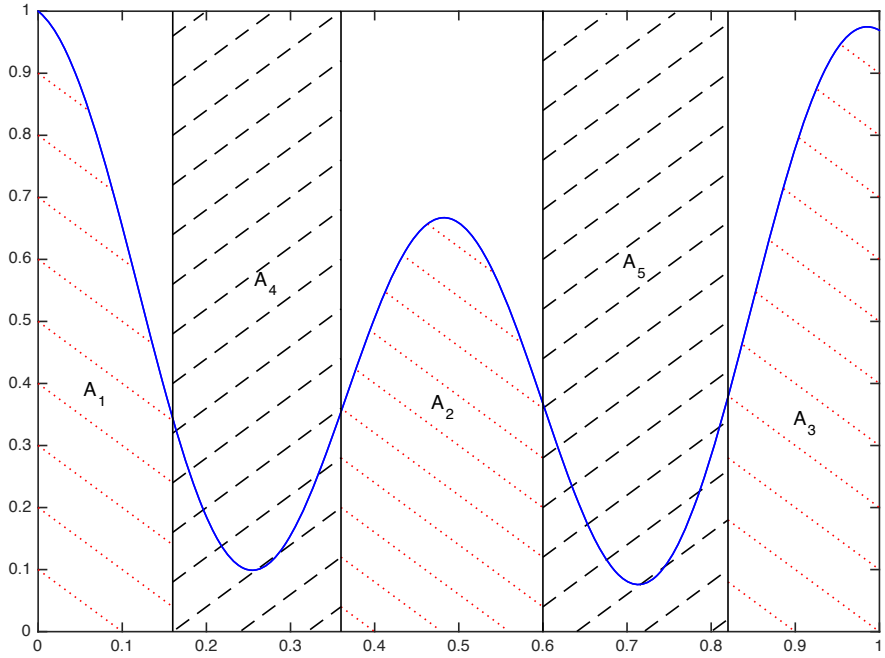


Figure 3.4: A pseudo-convex set in the unit square given by the area below graph of the density function and its admissible convex covering $A_i, i = 1, \ldots, 5$.

2. $A \subseteq (A_1 \cup \cdots \cup A_p)$,

3. *either* A_j *is a convex part of* A ($A_j \subseteq A$ *for* $j = 1, \ldots, q$) *or the complement of* A *with respect to* A_j, $A'_j = A_j \backslash A$ *is convex.*

Then A *is called a pseudo-convex set and* $A_1, \ldots, A_p$ *is an admissible convex covering for* A *with* p *parts and with* q *convex parts of* A.

Figure 3.4 shows a pseudo-convex set in the unit square given by the area below graph of the density function and its admissible convex covering. Let A be given by the graph under the curve. Then $A_i, i = 1, \ldots, 5$, is an admissible convex covering of A, where A_1, A_2 and A_3 are convex parts in A but A_4 and A_5 are rectangles shadowed region covering the remaining part of A. The regions $A_4 \backslash A$ and $A_5 \backslash A$ are convex.

Remark. *For convenience, we call a non-negative function pseudo-convex if and only if the region below its graph is a pseudo-convex set.*

Next we present a bound on the isotropic discrepancy of points generated by (t, m, s)-nets. A detailed proof is given in Section 3.6.1.

Lemma 3.1.7. *Let the point set $Q_{m,s} = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{M-1}\} \subseteq [0,1]^s$ be a (t, m, s)-net in base b where $M = b^m$. For the isotropic discrepancy of $Q_{m,s}$ we have*

$$J_M(Q_{m,s}) \leq 2sb^{t/s} M^{-1/s}.$$

A slightly weaker result than Lemma 3.1.7 can also be obtained from [61, Korollar 3].

Lemma 3.1.8. *For any point set P_N in $[0,1]^s$ we have*

$$J_N(P_N) \leq 2s \left(\frac{4s}{s-1}\right)^{(s-1)/s} (D_N^*(P_N))^{1/s}.$$

Further it is known from [47] that the star-discrepancy of a (t, m, s)-net $Q_{m,s}$ in base b, where $M = b^m$, satisfies

$$D_M^*(Q_{m,s}) \leq M^{-1} b^t (\log M)^{s-1} \frac{b^s}{(b+1)2^s (s-1)! (\log b)^{s-1}} + C_s M^{-1} b^t (\log M)^{s-2},$$

for some constant $C_s > 0$. These two inequalities therefore yield a convergence rate of order $M^{-1/s}(\log M)^{1-1/s}$.

The following lemma will be used to get a discrepancy bound for a point set on a pseudo-convex set. It is an extension of [1, Lemma 5] to the s-dimensional unit cube.

Lemma 3.1.9. *Let A be a pseudo-convex subset of $[0,1]^s$ with admissible convex covering of p parts with q convex parts of A. Then for any point set $P_N = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N-1}\} \subseteq [0,1]^s$ we have*

$$\left| \frac{1}{N} \sum_{n=0}^{N-1} 1_A(\boldsymbol{x}_n) - \lambda(A) \right| \leq (2p - q) J_N(P_N).$$

3.2 Discrepancy bounds

The first result we get is a discrepancy bound with respect to the target density of samples generated by the acceptance-rejection algorithm with deterministic driver sequences. The star-discrepancy of points generated by the acceptance-rejection algorithm with respect to the target density converges at the rate of $N^{-1/s}$, where N is the number of accepted samples. See Theorem 3.2.3 for details. The proof uses a bound on the discrepancy of our driver sequence with respect to convex sets (which is called isotropic discrepancy, see Definition 3.1.5 for details).

In order to investigate the discrepancy properties of samples obtained by the deterministic acceptance-rejection sampler, we first need to extend the concept of discrepancy to non-uniform distributions. The definition of the star-discrepancy of a sample set with respect to a density function ψ is given as follows.

Definition 3.2.1. *Let $\psi : [0,1]^{s-1} \to \mathbb{R}_+$ be an unnormalized target density with $C = \int_{[0,1]^{s-1}} \psi(\boldsymbol{z}) d\boldsymbol{z} > 0$. Let $Y_N^{(s-1)} = \{\boldsymbol{y}_0, \boldsymbol{y}_1, \ldots, \boldsymbol{y}_{N-1}\}$ be a point set in $[0,1]^{s-1}$. The star-discrepancy of $Y_N^{(s-1)}$ with respect to the density ψ defined in $[0,1]^{s-1}$ is defined by*

$$D^*_{N,\psi}(Y_N^{(s-1)}) = \sup_{\boldsymbol{t} \in [0,1]^{s-1}} \left| \frac{1}{N} \sum_{n=0}^{N-1} 1_{[\boldsymbol{0},\boldsymbol{t})}(\boldsymbol{y}_n) - \frac{1}{C} \int_{[\boldsymbol{0},\boldsymbol{t})} \psi(\boldsymbol{z}) d\boldsymbol{z} \right|,$$

where $[\boldsymbol{0},\boldsymbol{t}) = \prod_{j=1}^{s-1} [0, t_j)$.

Remark. *Note that ψ/C is a probability density function on $[0,1]^{s-1}$. Thus the discrepancy in the above Definition 3.2.1 measures the difference between the distribution ψ/C and the empirical distribution of the sample points with respect to the test sets $[\boldsymbol{0},\boldsymbol{t})$ for $\boldsymbol{t} \in [0,1]^{s-1}$.*

We consider now the induced star-discrepancy for the driver sequence from an acceptance-rejection sampler. In Definition 3.2.1 we defined the star-discrepancy with respect to th measure ψ/C. Assume that L is such that $\psi(\boldsymbol{x}) \leq L$ all $\boldsymbol{x} \in [0,1]^{s-1}$. We accept those points of the driver sequence $\{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{M-1}\} \subseteq [0,1]^s$

for which $\psi(x_{n,1}, \ldots, x_{n,s-1}) \geq Lx_{n,s}$ where $\boldsymbol{x}_n = (x_{n,1}, \ldots, x_{n,s})$. Thus the test sets for the driver sequence are of the form

$$\{\boldsymbol{x} \in [0,1]^s : (x_1, \ldots, x_{s-1}) \in [\mathbf{0}, \boldsymbol{t}),\ \psi(x_1, \ldots, x_{s-1}) \geq Lx_s\}.$$

See Figure 3.5 for an illustration for $s = 2$.

Compared with the classical definition of discrepancy, the test sets have changed from rectangles to intersections of rectangles with the graph under the target density which can be observed from Figure 3.5 If the target density is complicated in some sense, the test sets will end up with more irregular shape, which increases the difficulties for estimating the discrepancy. But under certain conditions, we can still obtain an estimation of the discrepancy.

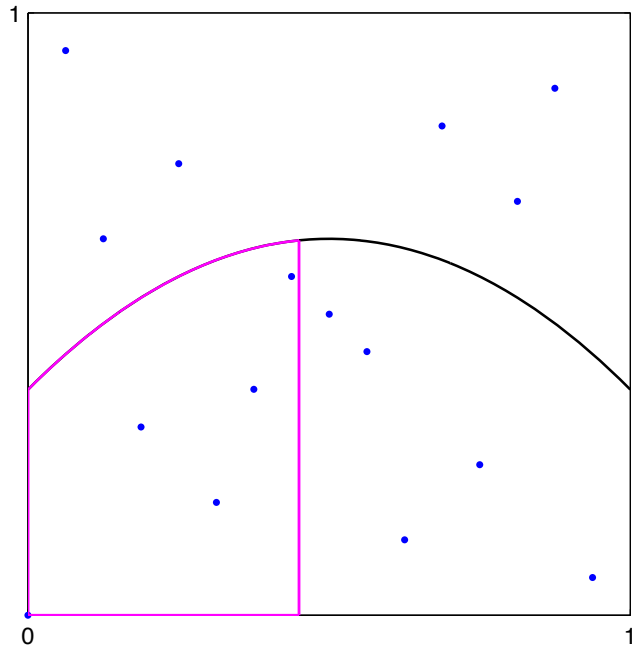


Figure 3.5: A test set in the local discrepancy with respect to a non-uniform measure.

3.2.1 Upper bound

Let an unnormalized density function $\psi : [0,1]^{s-1} \to \mathbb{R}_+$ be pseudo-convex, and $\int_{[0,1]^{s-1}} \psi(\boldsymbol{z}) d\boldsymbol{z} > 0$, but not necessarily 1. Assume that there exists a constant $L < \infty$ such that $\psi(\boldsymbol{x}) \leq L$ for all $\boldsymbol{x} \in [0,1]^{s-1}$. Let the subset under the graph of ψ/L be defined as

$$A = \{\boldsymbol{x} \in [0,1]^s : \psi(x_1, \ldots, x_{s-1}) \geq L x_s\}, \tag{3.2.1}$$

which is pseudo-convex in $[0,1]^s$ as ψ is a pseudo-convex function. Assume that there is an admissible convex covering of A with p parts and with q convex parts of A. Without loss of generality, let $A_1, \ldots, A_q$ be the convex subsets of A and $A_{q+1}, \ldots, A_p$, such that $A'_j = A_j \backslash A$ is convex for $q+1 \leq j \leq p$.

We consider now the case where the target density is defined on $[0,1]^{s-1}$. The following algorithm is a deterministic version of Algorithm 2.4.1. For the proofs later, we need the technical assumption that the target density is pseudo-convex (see the definition of pseudo-convexity in Definition 3.1.6).

Algorithm 3.2.2. *(Deterministic acceptance-rejection algorithm in $[0,1]^s$ based on (t,m,s)-nets). Let the target density $\psi : [0,1]^{s-1} \to \mathbb{R}_+$, where $s \geq 2$, be pseudo-convex. Assume that there exists a constant $L < \infty$ such that $\psi(\boldsymbol{x}) \leq L$ for all $\boldsymbol{x} \in [0,1]^{s-1}$. Let $A = \{\boldsymbol{x} \in [0,1]^s : \psi(x_1, \ldots, x_{s-1}) \geq L x_s\}$. Suppose we aim to obtain approximately N samples from ψ.*

i) Let $M = b^m \geq \left\lceil N / (\int_{[0,1]^{s-1}} \psi(\boldsymbol{x})/L d\boldsymbol{x}) \right\rceil$, where $m \in \mathbb{N}$ is the smallest integer satisfying this inequality. Generate a (t,m,s)-net $Q_{m,s} = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{b^m-1}\}$ in base b.

ii) Use the acceptance-rejection method for the points $Q_{m,s}$ with respect to the density ψ, i.e. we accept the point $\boldsymbol{x}_n$ if $\boldsymbol{x}_n \in A$, otherwise reject. Let $Y_N^{(s)} = A \cap Q_{m,s} = \{\boldsymbol{z}_0, \boldsymbol{z}_1, \ldots, \boldsymbol{z}_{N-1}\}$ be the sample set we accept.

iii) *Project the points* $P_N^{(s)}$ *onto the first* $(s-1)$ *coordinates.*
Let $Y_N^{(s-1)} = \{\boldsymbol{y}_0, \boldsymbol{y}_1, \ldots, \boldsymbol{y}_{N-1}\} \subseteq [0,1]^{s-1}$ *be the projections of the points* $Y_N^{(s)}$.

iv) *Return the point set* $Y_N^{(s-1)}$.

For the samples generated by this algorithm, we can prove the following upper bound on the star-discrepancy.

Theorem 3.2.3. *Let the unnormalized density function* $\psi : [0,1]^{s-1} \to \mathbb{R}_+$, *with* $s \geq 2$, *be pseudo-convex. Assume that there is an admissible convex covering of* A *given by Equation* (3.2.1) *with* p *parts and with* q *convex parts of* A. *Then the discrepancy of the point set* $Y_N^{(s-1)} = \{\boldsymbol{y}_0, \boldsymbol{y}_1, \ldots, \boldsymbol{y}_{N-1}\} \subseteq [0,1]^{s-1}$ *generated by Algorithm 3.2.2 using a* (t, s)*-sequence in base* b, *for large enough* N, *satisfies*

$$D^*_{N,\psi}(Y_N^{(s-1)}) \leq 8C^{-1}Lsb^{t/s}(2p-q)N^{-1/s},$$

where $C = \int_{[0,1]^{s-1}} \psi(\boldsymbol{z})d\boldsymbol{z}$ *and* $\psi(\boldsymbol{x}) \leq L$ *for all* $\boldsymbol{x} \in [0,1]^{s-1}$.

We postpone the proof of this theorem to Section 3.6.1.

3.2.2 Lower bound

In this section, we provide a lower bound on the star-discrepancy with respect to a concave density function. The general idea is to find, for a given driver point set, a density function satisfying a certain convergence rate.

Theorem 3.2.4. *Let* P_M *be an arbitrary point set in* $[0,1]^s$. *Then there exists a concave density function* ψ *defined on* $[0,1]^{s-1}$ *such that, for* N *samples generated by the acceptance-rejection algorithm with respect to* P_M *and* ψ, *we have*

$$D^*_{N,\psi}(P_N) \geq c_s N^{-\frac{2}{s+1}},$$

where $c_s > 0$ *is independent of* N *and the driver sequence* P_M *but depends on* s.

A detailed proof is provided in Section 3.6.2. We would like to point out that the lower bound also limits the convergence rate which we can obtain in our current approach via convex sets.

Additionally, note that [7] (in dimension $s = 2$) and [78] (for dimension $s > 2$) showed the existence of points with discrepancy with respect to convex sets bounded from above by $N^{-2/(s+1)}(\log N)^{c(s)}$ (where $c(s)$ is a function of only s). This would yield an improvement of our results from $N^{-1/s}$ to $N^{-2/(s+1)}(\log N)^{c(s)}$, however, those constructions are not explicit and can therefore not be used in computation.

3.2.3 Generalization to real state space

We consider now the case where the target density is defined on $\mathbb{R}^{s-1}$ with $s \geq 2$. The aim is to show a discrepancy bound on samples generated by the deterministic acceptance-rejection method. The discrepancy with respect to a given density function $\psi : \mathbb{R}^{s-1} \to \mathbb{R}_+$ is defined as follows.

Definition 3.2.5. *Let $Y_N^{(s-1)} = \{\boldsymbol{y}_0, \boldsymbol{y}_1, \ldots, \boldsymbol{y}_{N-1}\}$ be a point set in $\mathbb{R}^{s-1}$. Let $\psi : \mathbb{R}^{s-1} \to \mathbb{R}_+$ be an unnormalized probability density function. Then the star-discrepancy $D^*_{N,\psi}(Y_N^{(s-1)})$ is defined by*

$$D^*_{N,\psi}(Y_N^{(s-1)}) = \sup_{\boldsymbol{t} \in \mathbb{R}^{s-1}} \left| \frac{1}{N} \sum_{n=0}^{N-1} 1_{(-\boldsymbol{\infty}, \boldsymbol{t}]}(\boldsymbol{y}_n) - \frac{1}{C} \int_{(-\boldsymbol{\infty}, \boldsymbol{t}]} \psi(\boldsymbol{z}) d\boldsymbol{z} \right|,$$

where $C = \int_{\mathbb{R}^{s-1}} \psi(\boldsymbol{z}) d\boldsymbol{z}$ and $(-\boldsymbol{\infty}, \boldsymbol{t}] = \prod_{j=1}^{s-1}(-\infty, t_j]$ for $\boldsymbol{t} = (t_1, \ldots, t_{s-1})$.

The inverse Rosenblatt transformation is used to generate samples from the proposal density in the real state space $\mathbb{R}^{s-1}$. Let F be the joint CDF of H and $F_j(z_j | z_1, \ldots, z_{j-1})$ be the conditional CDF of the proposal density for $j = 1, \ldots, s-1$. The transformation T is used to generate points in $\mathbb{R}^{s-1} \times \mathbb{R}_+$ from the unit cube $[0,1]^s$, such that the projection of points onto the first $s-1$ coordinates has

distribution H. More precisely, let $T : [0,1]^s \to \mathbb{R}^s$ be the transformation given by

$$\boldsymbol{z} = T(\boldsymbol{u}) = \begin{cases} z_1 = F_1^{-1}(u_1), \\ z_j = F_j^{-1}(u_j | u_1, \ldots, u_{j-1}), \ 2 \leq j \leq s-1, \\ z_s = u_s H(z_1, \ldots, z_{s-1}). \end{cases} \tag{3.2.2}$$

The first $s-1$ coordinates are produced by the inverse Rosenblatt transformation which converts the points from the unit cube $[0,1]^{s-1}$ into $\mathbb{R}^{s-1}$. The sth coordinate is uniformly distributed on the line

$$\Big\{(1-v)(z_1, \ldots, z_{s-1}, 0) + v(z_1, \ldots, z_{s-1}, H(z_1, \ldots, z_{s-1})), 0 \leq v \leq 1\Big\}$$

if u_s is uniformly distributed in $[0,1]$. More details with respect to the Rosenblatt transformation and extensions can be found in [17, 72].

With the Rosenblatt transformation, the deterministic acceptance-rejection algorithm in $\mathbb{R}^s$ employing digital nets is conducted as follows.

Algorithm 3.2.6. *(Deterministic acceptance-rejection algorithm in $\mathbb{R}^s$ based on (t, m, s)-nets). Let an unnormalized target density function $\psi : \mathbb{R}^{s-1} \to \mathbb{R}_+$, where $s \geq 2$, be given. Let H be a proposal density $H : \mathbb{R}^{s-1} \to \mathbb{R}_+$, such that there exists a constant $L < \infty$ such that $\psi(\boldsymbol{z}) \leq LH(\boldsymbol{z})$ for all $\boldsymbol{z} \in \mathbb{R}^{s-1}$. Let $A = \{\boldsymbol{z} \in \mathbb{R}^s : \psi(z_1, \ldots, z_{s-1}) \geq LH(z_1, \ldots, z_{s-1})z_s\}$. Suppose we aim to obtain approximately N samples from ψ.*

i) Let $M = b^m \geq \left\lceil N \int_{[0,1]^{s-1}} H(\boldsymbol{x})d\boldsymbol{x} / (\int_{[0,1]^{s-1}} \psi(\boldsymbol{x})/Ld\boldsymbol{x}) \right\rceil$, where $m \in \mathbb{N}$ is the smallest integer satisfying this inequality. Generate a (t, m, s)-net $Q_{m,s} = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{M-1}\}$ in base b.

ii) Transform the points into $\mathbb{R}^{s-1} \times \mathbb{R}_+$ from $[0,1]^s$ using the transformation T given in (3.2.2) to obtain $\{T(\boldsymbol{x}_0), T(\boldsymbol{x}_1), \ldots, T(\boldsymbol{x}_{M-1})\}$.

iii) Take the acceptance-rejection method for the sample $T(\boldsymbol{x}_n)$ with respect to H and ψ in $\mathbb{R}^{s-1} \times \mathbb{R}_+$, i.e. accept the point $T(\boldsymbol{x}_n)$ if $T(\boldsymbol{x}_n) \in A$, otherwise reject. Let $Y_N^{(s)} = A \cap T(Q_{m,s}) = \{\boldsymbol{z}_0, \boldsymbol{z}_1, \ldots, \boldsymbol{z}_{N-1}\}$.

iv) Project the points $Y_N^{(s)}$ *we accepted onto the first* $(s-1)$*-dimensional space. Denote the point set obtained by projecting the accepted points onto the first* $s-1$ *coordinates by* $Y_N^{(s-1)} = \{\boldsymbol{y}_0, \boldsymbol{y}_1, \ldots, \boldsymbol{y}_{N-1}\} \subseteq \mathbb{R}^{s-1}$.

v) Return the point set $Y_N^{(s-1)}$.

We use the transformation T given in Equation (3.2.2) to generate samples of H. For the sake of investigating the discrepancy, the following result is helpful. The lemma shows that the transformation T and its inversion T^{-1} are both measure-preserving. For the proofs later, we assume that the proposal density H is a product measure, i.e. $H = \prod_{j=1}^{s-1} H_j$, where H_j is the marginal density with respect to z_j. In our numerical examples, the proposal density is not necessarily of product type.

Lemma 3.2.7. *The transformation* T *from the* s*-dimensional unit cube to* $\mathbb{R}^{s-1} \times \mathbb{R}_+$ *given in Equation* (3.2.2) *is measure-preserving, i.e.* $Volume(T(D)) = Volume(D)$ *holds for any measurable set* $D \subseteq [0,1]^s$. *This is true for* T^{-1} *as well.*

To prove a bound on the discrepancy of the samples generated by Algorithm 3.2.6, the following assumption is needed.

Assumption 1. *Let* ψ *be the target density and* H *be a product measure proposal density function, which is chosen such that its inverse CDF can be computed. Let* $A = \{\boldsymbol{z} \in \mathbb{R}^s : \psi(z_1, \ldots, z_{s-1}) \geq L z_s H(z_1, \ldots, z_{s-1})\}$ *and the transformation* T^{-1} *is defined as the inversion of the transform* T. *Then we assume that* $T^{-1}(A)$ *is pseudo-convex.*

As the mappings T and T^{-1} are measure preserving, and since there are the same number of samples in an arbitrary subset $D \subseteq [0,1]^s$ and the corresponding subset $T(D) \subseteq \mathbb{R}^{s-1} \times \mathbb{R}_+$, we can consider the discrepancy in the unit cube instead of that in $\mathbb{R}^{s-1} \times \mathbb{R}_+$. Following similar arguments as for Theorem 3.2.3 and Theorem 3.2.4, we obtain the same discrepancy bounds including an upper bound and a lower bound for the general density ψ defined in the real state space $\mathbb{R}^{s-1}$.

Theorem 3.2.8. *Let the unnormalized target density $\psi : \mathbb{R}^{s-1} \to \mathbb{R}_+$ and the proposal density $H : \mathbb{R}^{s-1} \to \mathbb{R}_+$ satisfy Assumption 1. Then the discrepancy of the point set $Y_N^{(s-1)} = \{\boldsymbol{y}_0, \boldsymbol{y}_1, \dots, \boldsymbol{y}_{N-1}\} \subseteq \mathbb{R}^{s-1}$ generated by Algorithm 3.2.6 satisfies*

$$D^*_{N,\psi}(Y_N^{(s-1)}) \leq 8LC^{-1}sb^{t/s}(2p-q)N^{-1/s},$$

for N large enough, where $C = \int_{\mathbb{R}^{s-1}} \psi(\boldsymbol{z})d\boldsymbol{z} > 0$ and L is such that $\psi(\boldsymbol{x}) \leq LH(\boldsymbol{x})$ for all $\boldsymbol{x} \in \mathbb{R}^{s-1}$.

Theorem 3.2.9. *Let H be a product density function defined on $\mathbb{R}^{s-1}$. Let T be the transformation given in Equation (3.2.2) associated with H. Let P_M be an arbitrary point set in $[0,1]^s$, then $T(P_M)$ is a point set in $\mathbb{R}^{s-1}$. Then there exists an unnormalized density function ψ defined in $\mathbb{R}^{s-1}$ satisfying the assumption in Theorem 3.2.8 such that the star-discrepancy of the points generated by the acceptance-rejection sampler with respect to ψ and H satisfies*

$$D^*_{N,\psi}(Y_N^{(s-1)}) \geq c_s N^{-\frac{2}{s+1}},$$

where c_s is independent of N and P_M, but depends on s.

3.2.4 An improved upper bound

In this section we prove a convergence rate of order $N^{-\alpha}$ for $1/s \leq \alpha < 1$, where α depends on the target density ψ. See Theorem 3.2.12 below for details. For this result we use (t, m, s)-nets (see Definition 3.1.3 below) as inputs. The value of α here depends on how well the graph of ψ can be covered by certain rectangles (see Equation (3.2.3)). In practice this covering rate of order $N^{-\alpha}$ is hard to determine precisely, α arbitrarily close to 1 can be achieved if ψ is constant. We also provide a simple example in dimension $s = 2$ for which α can take on the values $\alpha = 1 - \ell^{-1}$ for $\ell = 2, 3, \dots$. See Example 3.2.13 for details.

We use the acceptance-rejection algorithm based on (t, m, s)-nets in base b as driver sequence formalized in Algorithm 3.2.2. Let again $Y_N^{(s-1)} = \{\boldsymbol{y}_0, \boldsymbol{y}_1, \dots, \boldsymbol{y}_{N-1}\} \subseteq [0,1]^{s-1}$ be the accepted point set.

In the following we show that an improvement of the discrepancy bound for the deterministic acceptance-rejection sampler is possible in some special cases. Let an unnormalized density function $\psi : [0,1]^{s-1} \to \mathbb{R}_+$, with $s \geq 2$, be given. Let again

$$A = \{\boldsymbol{z} = (z_1, \ldots, z_s) \in [0,1]^s : \psi(z_1, \ldots, z_{s-1}) \geq L z_s\}$$

and $J_{\boldsymbol{t}}^* = ([\boldsymbol{0}, \boldsymbol{t}) \times [0,1]) \bigcap A$. Let $\partial J_{\boldsymbol{t}}^*$ denote the boundary of $J_{\boldsymbol{t}}^*$ and $\partial [0,1]^s$ denote the boundary of $[0,1]^s$. For $k \in \mathbb{N}$ we define the covering number

$$\Gamma_k(\psi) = \sup_{\boldsymbol{t} \in [0,1]^s} \min\{v : \exists U_1, \ldots, U_v \in \mathcal{E}_k : (\partial J_{\boldsymbol{t}}^* \setminus \partial [0,1]^s) \subseteq \bigcup_{i=1}^{v} U_i, \\ U_i \cap U_{i'} = \emptyset \text{ for } 1 \leq i < i' \leq v\}, \tag{3.2.3}$$

where $\mathcal{E}_k$ is the family of elementary intervals of order k.

Lemma 3.2.10. *Let $\psi : [0,1]^{s-1} \to [0,1]$ be an unnormalized target density and let the covering number $\Gamma_{m-t}(\psi)$ be given by (3.2.3). Then the discrepancy of the point set $Y_N^{(s-1)} = \{\boldsymbol{y}_0, \boldsymbol{y}_1, \ldots, \boldsymbol{y}_{N-1}\} \subseteq [0,1]^{s-1}$ generated by the deterministic acceptance-rejection sampler using a (t, m, s)-net in base b, for large enough N, satisfies*

$$D_{N,\psi}^*(Y_N^{(s-1)}) \leq 4 C^{-1} b^t \Gamma_{m-t}(\psi) N^{-1},$$

where $C = \int_{[0,1]^{s-1}} \psi(\boldsymbol{z}) d\boldsymbol{z} > 0$.

We postpone the proof of Lemma 3.2.10 to Section 3.6.3. To obtain a bound on the discrepancy, we need to further estimate the covering number. The covering number $\Gamma_{m-t}(\psi)$ is difficult to estimate in general, but can be estimated for special cases. A known example is the following. Assume that ψ is constant. Since the graph of ψ can be covered by just one elementary interval of order $m-t$, this is the simplest possible case. The results from [59, Section 3] (see also [23, pp. 184–190] for an exposition in dimensions $s = 1, 2, 3$) imply that $\Gamma_k(\psi) \leq C_s k^{s-1}$ for some constant C_s which depends only on s. This yields the convergence rate of order $(\log N)^{s-1} N^{-1}$ in Lemma 3.2.10.

In order to prove an improved bound on the star discrepancy, for the requirement of our proof techniques, we assume that the set below the graph of the density function admits a so-called Minkowski content.

Definition 3.2.11. *(Minkowski content). For a set $A \subseteq \mathbb{R}^s$, let ∂A denote the boundary of A and let*

$$\mathcal{M}(\partial A) = \lim_{\varepsilon \to 0} \frac{\lambda((\partial A)_\varepsilon)}{2\varepsilon},$$

where $(\partial A)_\varepsilon = \{\boldsymbol{x} \in \mathbb{R}^s | \|\boldsymbol{x} - \boldsymbol{y}\| \leq \varepsilon \text{ for } \boldsymbol{y} \in \partial A\}$ and $\|\cdot\|$ denotes the Euclidean norm. If $\mathcal{M}(\partial A)$ (abbreviated as $\mathcal{M}_A$) exists and is finite, then ∂A is said to admit an $(s-1)-$dimensional Minkowski content.

For simplicity, we consider the Minkowski content associated with the boundary of a given set, however one could define it in a more general sense. Ambrosio et al [4] present a detailed discussion of general Minkowski content.

Following the above discussion, in general, there are constants $c_{s,\psi}$ and $C_{s,\psi}$ depending only on s and ψ such that

$$c_{s,\psi} k^{s-1} \leq \Gamma_k(\psi) \leq C_{s,\psi} b^{(1-1/s)k}, \tag{3.2.4}$$

whenever the set ∂A admits an $(s-1)-$dimensional Minkowski content. This yields a convergence rate in Lemma 3.2.10 of order $N^{-\alpha}$ with $1/s \leq \alpha < 1$, where the precise value of α depends on ψ. We obtain the following result.

Theorem 3.2.12. *Let $\psi : [0,1]^{s-1} \to [0,1]$ be an unnormalized target density and let $\Gamma_k(\psi)$ be given by (3.2.3). Assume that there is a constant $\Theta > 0$ such that*

$$\Gamma_k(\psi) \leq \Theta b^{(1-\alpha)k} k^\beta \quad \text{for all } k \in \mathbb{N},$$

for some $1/s \leq \alpha < 1$ and $\beta \geq 0$. Then there is a constant $\Delta_{s,t,\psi} > 0$ which depends only on s, t and ψ, such that the discrepancy of the point set $Y_N^{(s-1)} = \{\boldsymbol{y}_0, \boldsymbol{y}_1, \ldots, \boldsymbol{y}_{N-1}\} \subseteq [0,1]^{s-1}$ generated by the deterministic acceptance-rejection sampler using a (t, m, s)-net in base b, for large enough N, satisfies

$$D^*_{N,\psi}(Y_N^{(s-1)}) \leq \Delta_{s,t,\psi} N^{-\alpha} (\log N)^\beta.$$

Remark. *Note that a finite covering number $\Gamma_k(\psi)$ ensures the existence of $(s-1)$-dimensional Minkowski content.*

Example 3.2.13. *To illustrate the bound in Theorem 3.2.12, we consider now an example for which we can obtain an explicit bound on $\Gamma_k(\psi)$ of order $b^{k(1-\alpha)}$ for $1/2 \le \alpha < 1$. For simplicity let $s = 2$ and $\alpha = 1 - \ell^{-1}$ for some $\ell \in \mathbb{N}$ with $\ell \ge 2$. We define now a function $\psi_\ell : [0,1) \to [0,1)$ in the following way: let $x \in [0,1)$ have b-adic expansion*

$$x = \frac{\xi_1}{b} + \frac{\xi_2}{b^2} + \frac{\xi_3}{b^3} + \cdots$$

where $\xi_i \in \{0, 1, \ldots, b-1\}$ and assume that infinitely many of the ξ_i are different from $b-1$. Then set

$$\psi_\ell(x) = \frac{\xi_1}{b^{l-1}} + \frac{\xi_2}{b^{2(l-1)}} + \frac{\xi_3}{b^{3(l-1)}} + \cdots .$$

Let $t \in [0,1)$. In the following we define elementary intervals of order $k \in \mathbb{N}$ which cover $\partial J_{\boldsymbol{t}}^* \setminus \partial[0,1]^2$. Assume first that k is a multiple of ℓ, then let $g = k/\ell$. Then we define the following elementary intervals of order $k = g\ell$:

$$\left[\frac{a_1}{b} + \cdots + \frac{a_{g-1}}{b^{g-1}} + \frac{a_g}{b^g}, \frac{a_1}{b} + \cdots + \frac{a_{g-1}}{b^{g-1}} + \frac{a_g+1}{b^g}\right) \times \left[\frac{a_1}{b^{\ell-1}} + \cdots + \frac{a_{g-1}}{b^{(g-1)(\ell-1)}} + \frac{a_g}{b^{g(\ell-1)}}, \frac{a_1}{b^{\ell-1}} + \cdots + \frac{a_{g-1}}{b^{(g-1)(\ell-1)}} + \frac{a_g+1}{b^{g(\ell-1)}}\right), \tag{3.2.5}$$

where $a_1, \ldots, a_g \in \{0, 1, \ldots, b-1\}$ run through all possible choices such that

$$\frac{a_1}{b} + \cdots + \frac{a_{g-1}}{b^{g-1}} + \frac{a_g+1}{b^g} \le t.$$

The number of these choices for $a_1, \ldots, a_g$ is bounded by b^g. Let

$$t = \frac{t_1}{b} + \cdots + \frac{t_g}{b^g} + \frac{t_{g+1}}{b^{g+1}} + \cdots .$$

For integers $1 \le u \le g(\ell-1)$ and $0 \le c_u < t_{g+u}$, we define the intervals

$$\left[\frac{t_1}{b} + \cdots + \frac{t_{g+u-1}}{b^{g+u-1}} + \frac{c_u}{b^{g+u}}, \frac{t_1}{b} + \cdots + \frac{t_{g+u-1}}{b^{g+u-1}} + \frac{c_u+1}{b^{g+u}}\right) \times \left[\frac{d_1}{b} + \cdots + \frac{d_{g(\ell-1)-u}}{b^{g(\ell-1)-u}}, \frac{d_1}{b} + \cdots + \frac{d_{g(\ell-1)-u}}{b^{g(\ell-1)-u}} + \frac{1}{b^{g(\ell-1)-u}}\right), \tag{3.2.6}$$

where $d_i = 0$ *if* $\ell \nmid i$, $d_i = t_{i/\ell}$ *if* $\ell | i$ *and we set* $\frac{d_1}{b} + \cdots + \frac{d_{g(\ell-1)-u}}{b^{g(\ell-1)-u}} = 0$ *if* $u = g(\ell - 1)$. *Further we define the interval*

$$\left[\frac{t_1}{b} + \cdots + \frac{t_{g\ell}}{b^{g\ell}}, \frac{t_1}{b} + \cdots + \frac{t_{g\ell}}{b^{g\ell}} + \frac{1}{b^{g\ell}}\right) \times [0, 1). \tag{3.2.7}$$

The intervals defined in (3.2.5), (3.2.6) *and* (3.2.7) *cover* $\partial J_t^* \setminus \partial[0,1]^2$. *Thus we have*

$$\Gamma_{g\ell}(\psi_\ell) \leq b^g + bg(\ell - 1) + 1 \leq \ell b^g.$$

For arbitrary $k \in \mathbb{N}$ *we can use elementary intervals of order* k *which cover the same area as the intervals* (3.2.5), (3.2.6) *and* (3.2.7). *Thus we have at most* $b^{\ell-1}$ *times as many intervals and we therefore obtain*

$$\Gamma_k(\psi_\ell) \leq \ell b^{k/\ell + \ell - 1}.$$

Thus we obtain

$$\sup_{t \in [0,1]} \left| \frac{1}{N} \sum_{n=0}^{N-1} 1_{[0,t)}(y_n) - \frac{1}{C} \int_0^t \psi_\ell(z)\, \mathrm{d}z \right| \leq \Delta_{s,t,\psi} N^{-(1-\frac{1}{\ell})}.$$

3.3 A deterministic reduced acceptance-rejection sampler

In this section we consider an extension of the deterministic acceptance-rejection sampler. The random version of this reduced method was recently introduced by Barekat and Caflisch in [6], where a reduced acceptance-rejection algorithm is used for kinetic simulation in which the rates are fluctuating in time and have singular limits, as occurs for example in simulation of recombination interactions in a plasma.

The basic idea is that for a target density function ψ, we carefully select H such that for $\psi - H$ and H the inverse CDF can be computed. For the case $\psi(\boldsymbol{x}) > H(\boldsymbol{x})$, we write $\psi = (\psi - H) + H$ and get samples according to $\psi - H$ and H respectively.

Figure 3.6 illustrates this method. The area under the graph of ψ can be divided into three subsets, $R_{1,1}, R_{1,2}$ and $R_{2,2}$, where samples with distribution according to the upper bound of $R_{1,2}$ and $R_{2,2}$ can be directly generated by using

the inverse CDF of H and $\psi - H$. The acceptance-rejection method is only used for the region $R_{1,1}$. Compared with the ordinary acceptance-rejection sampler, one obvious merit of this method is that we do not require $\psi(\boldsymbol{x}) \leq H(\boldsymbol{x})$ in the whole domain. Also, this method might give better convergence rates since samples with distribution according to the upper bound of $R_{1,2}$ and $R_{2,2}$ are obtained via inversion transform and therefore have low discrepancy. Algorithm 3.3.1 gives a simple version of the improved method. More discussion of a general version is available in Algorithms 3.3.2.

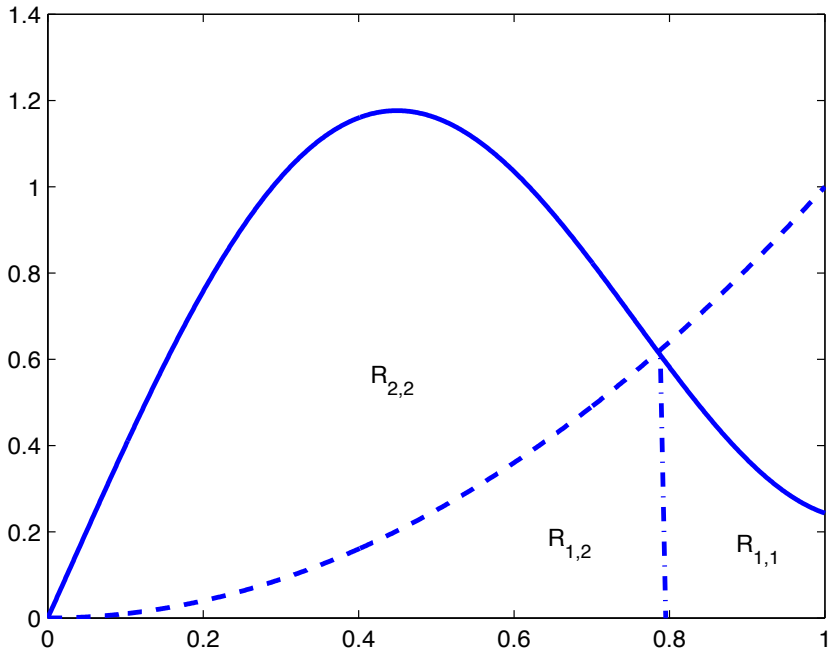


Figure 3.6: The idea of the reduced acceptance-rejection sampler, where the solid line represents the target density ψ and the dashed line is the proposal density H.

3.3.1 Algorithm

Now we present the quasi-Monte Carlo version of the reduced acceptance-rejection sampler for a simple case.

Algorithm 3.3.1. *(Deterministic reduced acceptance-rejection sampler based on (t, s)-sequence) Let $\psi : [0,1] \to \mathbb{R}_+$ be a target density. Choose a proposal density H such that $\psi - H$ and H can be sampled directly. Let*

$$\mathcal{S} := \{x \in [0,1] : \psi(x) < H(x)\},$$

and

$$\mathcal{L} := \{x \in [0,1] : \psi(x) \geq H(x)\}.$$

Assume that

$$\frac{\int_{\mathcal{S}} \psi(x)dx}{\int_{[0,1]} \psi(x)dx}, \quad \frac{\int_{\mathcal{L}} H(x)dx}{\int_{[0,1]} \psi(x)dx} \text{ and } \quad \frac{\int_{\mathcal{L}} (\psi - H)(x)dx}{\int_{[0,1]} \psi(x)dx}$$

can be calculated or estimated. Let $F^{-1}_{H,\mathcal{S}}, F^{-1}_{H,\mathcal{L}}$ be the inverse CDF of the proposal density H in the domain $\mathcal{S}$ and $\mathcal{L}$ respectively and $F^{-1}_{\psi-H,\mathcal{L}}$ be the inverse CDF with respect to $\psi - H$ in $\mathcal{L}$. Suppose we aim to generate approximately N samples from ψ. Let

$$N_1 = \left\lceil N \frac{\int_{\mathcal{S}} \psi(x)dx}{\int_{[0,1]} \psi(x)dx} \right\rceil, \; N_2 = \left\lceil N \frac{\int_{\mathcal{L}} H(x)dx}{\int_{[0,1]} \psi(x)dx} \right\rceil \text{ and } N_3 = \left\lceil N \frac{\int_{\mathcal{L}} (\psi - H)(x)dx}{\int_{[0,1]} \psi(x)dx} \right\rceil.$$

i) Let $\{\boldsymbol{x}_0, \boldsymbol{x}_1, \boldsymbol{x}_2, \ldots\} \subseteq [0,1]^2$ be a $(t, 2)$-sequence in base b.

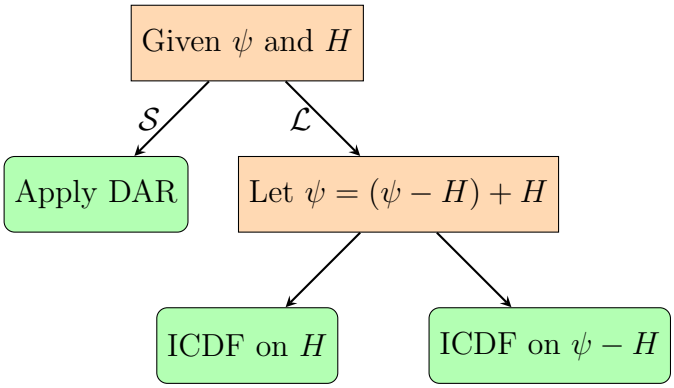
ii) Use the acceptance-rejection method with respect the target density ψ and the proposal density H on the domain $\mathcal{S}$ with $\{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{M-1}\}$ as driver sequence. Choose M such that N_1 points are accepted by the deterministic acceptance-rejection algorithm. Compute $F^{-1}_{H,\mathcal{S}}(\boldsymbol{x}_n)$ for $n = 0, 1, 2, \ldots, M-1$. Let $Y_{1,1} = \{\boldsymbol{z}_0, \boldsymbol{z}_1, \ldots, \boldsymbol{z}_{N_1-1}\}$ be the accepted point set.

iii) Compute the points $F^{-1}_{H,\mathcal{L}}(\boldsymbol{x}_n)$ for $n = 0, 1, \ldots, N_2 - 1$. Let $Y_{1,2} = \{F^{-1}_{H,\mathcal{L}}(\boldsymbol{x}_n) : 0 \leq n < N_2\}$.

iv) Compute the points $F^{-1}_{\psi-H,\mathcal{L}}(\boldsymbol{x}_n)$ for $n = 0, 1, \ldots, N_3 - 1$. Let $Y_{2,2} = \{F^{-1}_{\psi-H,\mathcal{L}}(\boldsymbol{x}_n) : 0 \leq n < N_3\}$.

v) Project the points in $Y_{1,1} \cup Y_{1,2} \cup Y_{2,2}$ onto the first coordinate to obtain the sample set Y_N in $[0,1]$. Return the point set Y_N.

To provide a better understanding, we use a simple flow chart below to illustrate the idea again for a target density ψ and the well-chosen proposal density H such that the inverse cumulative distribution function (ICDF) of $\psi - H$ and H are available in convenient forms, see also in [6]. Then deterministic acceptance-rejection (DAR) algorithm is used only for sampling from region $\mathcal{S}$.



Since the inverse transform is a measure-preserving transformation, it can preserve the uniformities of the driver sequence. Thus samples generated in $R_{1,2}$ and $R_{2,2}$ are low-discrepancy point sets. Example 3.5.3 verifies the efficiency of the deterministic acceptance-rejection algorithm. A theoretical result on the discrepancy properties of samples obtained by this class of algorithms will be provided in Theorem 3.3.3 below.

Algorithm 3.3.1 can be extended to a more general case. Consider the target density $\psi(\boldsymbol{x}) = \sum_{\ell=1}^{k} H_\ell(\boldsymbol{x}), \boldsymbol{x} \in D \subseteq \mathbb{R}^s$. If it is possible to sample from $H_\ell(\boldsymbol{x})$ individually and the expectations of H_ℓ can be calculated or estimated with low cost, then we can use an embedded deterministic reduced acceptance-rejection sampler in each step. Let

$$\mathcal{S}_\ell = \{\boldsymbol{x} \in D : \psi_{k-\ell+1}(\boldsymbol{x}) < H_\ell(\boldsymbol{x})\},$$

and

$$\mathcal{L}_\ell = \{\boldsymbol{x} \in D : \psi_{k-\ell+1}(\boldsymbol{x}) \geq H_\ell(\boldsymbol{x})\}, \tag{3.3.1}$$

where $\psi_{k-\ell+1}(\boldsymbol{x}) = \sum_{i=\ell}^{k} H_i(\boldsymbol{x})$ for $\ell = 1, \ldots, k-1$, and, in particular, ψ_k is the target density.

Suppose we aim to sample N points from the target density ψ. The sample set can be divided into two types, namely, points generated from the sets $\mathcal{S}_\ell$'s and $\mathcal{L}_\ell$'s respectively. We apply a deterministic acceptance-rejection method given in Algorithm 3.2.6 in each $\mathcal{S}_\ell$ with respect to $\psi_{k-\ell+1}$ and H_ℓ. Note that we get $\lceil N \int_{\mathcal{S}_\ell} \psi_{k-\ell+1}(\boldsymbol{x})d\boldsymbol{x} / \int_D \psi_k(\boldsymbol{x})d\boldsymbol{x} \rceil$ points from $\mathcal{S}_\ell$ for $\ell = 1, \ldots, k-1$. For sampling from $\mathcal{L}_\ell$, the remaining samples come from applying the inverse transformation of H_ℓ in $\mathcal{L}_\ell$. Then we obtain an additional $\lceil N \int_{\mathcal{L}_\ell} H_\ell(\boldsymbol{x})d\boldsymbol{x} / \int_D \psi_k(\boldsymbol{x})d\boldsymbol{x} \rceil$ points from $\mathcal{L}_\ell$ for $\ell = 1, \ldots, k$. We conduct the procedure inductively until we get samples from $H_k(\boldsymbol{x})$. We assume that $\int_{\mathcal{S}_\ell} \psi_{k-\ell+1}(\boldsymbol{x})d\boldsymbol{x} / \int_D \psi_k(\boldsymbol{x})d\boldsymbol{x}$ and $\int_{\mathcal{L}_\ell} H_\ell(\boldsymbol{x})d\boldsymbol{x} / \int_D \psi_k(\boldsymbol{x})d\boldsymbol{x}$ can be calculated or estimated.

The following algorithm is an extension of the simple algorithm, which summarizes the embedding idea.

Algorithm 3.3.2. *Let $\psi(\boldsymbol{x}) = \sum_{\ell=1}^{k} H_\ell(\boldsymbol{x}), \boldsymbol{x} \in D \subset \mathbb{R}^{s-1}$, be a target density we aim to sample from. Define $\psi_{k-\ell+1}(\boldsymbol{x}) = \sum_{i=\ell}^{k} H_i(\boldsymbol{x})$ for $j = 1, \ldots, k-1$. Let $\mathcal{S}_\ell$ and $\mathcal{L}_\ell$ be as in Equation (3.3.1) and assume that $\int_{\mathcal{S}_\ell} \psi_{k-\ell+1}(\boldsymbol{x})d\boldsymbol{x} / \int_D \psi(\boldsymbol{x})d\boldsymbol{x}$ and $\int_{\mathcal{L}_\ell} H_\ell(\boldsymbol{x})d\boldsymbol{x} / \int_D \psi(\boldsymbol{x})d\boldsymbol{x}$ can be calculated or estimated. Further assume that we can sample from H_ℓ individually by applying the transformation $T_{H_\ell,\mathcal{S}_\ell}$ and $T_{H_\ell,\mathcal{L}_\ell}$ given in Equation (3.2.2) in $\mathcal{S}_\ell$ and $\mathcal{L}_\ell$ respectively. Suppose we aim to generate N samples from ψ. Let*

$$N_{1,\ell} = \left\lceil N \frac{\int_{\mathcal{S}_\ell} \psi_{k-\ell+1}(\boldsymbol{x})d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x})d\boldsymbol{x}} \right\rceil \quad \text{and} \quad N_{2,j} = \left\lceil N \frac{\int_{\mathcal{L}_\ell} H_\ell(\boldsymbol{x})d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x})d\boldsymbol{x}} \right\rceil.$$

For ℓ from 1 to k do:

i) Let $\{\boldsymbol{x}_0, \boldsymbol{x}_1, \boldsymbol{x}_2, \ldots\} \subseteq [0,1]^s$ be a (t, s)-sequence in base b.

ii) Compute $T_{H_\ell,\mathcal{S}_\ell}(\boldsymbol{x}_n)$ for $n = 0, 1, 2, \ldots$. Use the acceptance-rejection method with respect to $\psi_{k-\ell+1}$ and H_ℓ on the domain $\mathcal{S}_\ell$ using $\{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{M-1}\}$ as driver sequence. Choose M such that $N_{1,\ell}$ points are accepted by the acceptance-rejection algorithm. Let $Y_{1,\ell}^{(s)} = \{\boldsymbol{z}_0, \boldsymbol{z}_1, \ldots, \boldsymbol{z}_{N_{1,\ell}-1}\}$ be the accepted points.

iii) *Compute* $T_{H_\ell,\mathcal{L}_\ell}(\boldsymbol{x}_n)$ *for* $n = 0, 1, \ldots, N_{2,\ell} - 1$. *Let* $Y_{2,\ell}^{(s)} = \{T_{H_\ell,\mathcal{L}_\ell}(\boldsymbol{x}_n) : 0 \leq n < N_{2,\ell}\}$.

Then let $Y_N^{(s)} = \bigcup_{\ell=1}^{k}(Y_{1,\ell}^{(s)} \cup Y_{2,\ell}^{(s)})$ *and let* $Y_N^{(s-1)}$ *denote the projection of* $Y_N^{(s)}$ *onto the first* $s-1$ *coordinates. Return the set* $Y_N^{(s-1)}$.

3.3.2 Discrepancy bounds for samples generated by the reduced acceptance-rejection sampler

Now we consider the discrepancy properties of sample points produced by this reduced acceptance-rejection algorithm. Note that the sample set of $\psi = \sum_{\ell=1}^{k} H_\ell$ can be decomposed into several subsets with different star-discrepancy. Similarly to the triangle inequality for the discrepancy presented in Proposition 2.1.4, we have a triangle inequality for the star-discrepancy with respect to a density function.

Theorem 3.3.3. *For a given target density* $\psi(\boldsymbol{x}) = \sum_{\ell=1}^{k} H_\ell(\boldsymbol{x}), \boldsymbol{x} \in D \subset \mathbb{R}^{s-1}$, *let* $\psi_{k-\ell+1}(\boldsymbol{x}) = \sum_{i=\ell}^{k} H_i(\boldsymbol{x})$. *Let* $\mathcal{S}_\ell$ *and* $\mathcal{L}_\ell$ *be given by* (3.3.1). *Let* $Y_N^{(s-1)}$ *be the sample set generated by Algorithm 3.3.2, where*

$$N_{1,\ell} = \left\lceil N \int_{\mathcal{S}_\ell} \psi_{k-\ell+1}(\boldsymbol{x}) d\boldsymbol{x} / \int_D \psi_k(\boldsymbol{x}) d\boldsymbol{x} \right\rceil,$$

which is the number of points generated from $\mathcal{S}_\ell$, *and*

$$N_{2,\ell} = \left\lceil N \int_{\mathcal{L}_\ell} H_\ell(\boldsymbol{x}) d\boldsymbol{x} / \int_D \psi_k(\boldsymbol{x}) d\boldsymbol{x} \right\rceil,$$

which is the number of points generated from $\mathcal{L}_\ell$ *for* $\ell = 1, \ldots, k$. *Assume that* $N_{1,\ell}$ *and* $N_{2,\ell}$ *can be calculated for the given target density* ψ *and* N. *Then we have*

$$D_{N,\psi}^*(Y_N^{(s-1)}) \leq \sum_{\ell=1}^{k-1} \frac{N_{1,\ell}}{N} D_{\mathcal{S}_\ell,\psi_{k-\ell+1}}^* + \sum_{\ell=1}^{k} \frac{N_{2,\ell}}{N} D_{\mathcal{L}_\ell,H_\ell}^* + \frac{1}{N},$$

where $D_{\mathcal{S}_\ell,\psi_{k-\ell+1}}^*$ *and* $D_{\mathcal{L}_\ell,H_\ell}^*$ *is the discrepancy of the samples in* $\mathcal{S}_\ell$ *and* $\mathcal{L}_\ell$ *respectively.*

The proof of Theorem 3.3.3 is given in Appendix 3.6.4. Note that this method achieves an improved acceptance rate of points compared with the plain acceptance-rejection algorithm for the target density ψ, since we are only rejecting points in a

certain range. For the remaining domain, we get samples by applying the inverse transform. To be more exact, all point sets from $\mathcal{L}_\ell$ have low discrepancy since the inverse transformation is directly applied with respect to H_ℓ for $\ell = 1, \dots, k$. Now we consider the star-discrepancy of points generated from $\mathcal{S}_\ell$.

The following result from [47] gives an improved upper bound of the star-discrepancy on the first M terms of a (t, s)-sequence in base b with $s \geq 2$.

Lemma 3.3.4. *The star-discrepancy of the first M terms Q_M of a (t, s)-sequence in base b with $s \geq 2$ satisfies*

$$D_M^*(Q_M) \leq M^{-1} b^t (\log M)^s \frac{b^s(b-1)}{(b+1)2^{s+1}(s!)(\log b)^s} + C_s M^{-1} b^t (\log M)^{s-1},$$

for some constant $C_s > 0$ only depending on s.

With the help of Lemma 3.1.8, we obtain a bound on the isotropic discrepancy of the first M points of a (t, s)-sequence.

Lemma 3.3.5. *Let the point set $Q_M = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \dots, \boldsymbol{x}_{M-1}\} \subset [0,1]^s$ be the first M terms of a (t, s)-sequence. For the isotropic discrepancy of Q_M we have*

$$J_M(Q_M) \leq 2s \left(\frac{4s}{s-1}\right)^{(s-1)/s} \left(\frac{b^{t/s} \left(\frac{b^s(b-1)}{(b+1)2^{s+1}(s!)(\log b)^s}\right)^{1/s} \log M}{M^{1/s}} + \frac{C_s' b^{t/s} (\log M)^{(s-1)/s}}{M^{1/s}} \right),$$

for some constant $C_s' > 0$ depending only on s.

Hence, for the star-discrepancy of $Y_{1,\ell}$ for $1 \leq \ell < k$, using a (t, s)-sequence as a driver sequence in the acceptance-rejection algorithm we have a convergence rate of order $N_{1,\ell}^{-1/s} \log N_{1,\ell}$. We omit a detailed proof since similar arguments as for proving Theorem 3.2.3 can be used. The following corollary holds by substituting the proper upper bounds and $N_{1,\ell}, N_{2,\ell}$ in terms of N.

Corollary 3.3.6. *Suppose that the target density $\psi(\boldsymbol{x}) = \sum_{\ell=1}^k H_\ell(\boldsymbol{x}), \boldsymbol{x} \in D \subset \mathbb{R}^{s-1}$ satisfies all assumptions stated in Theorem 3.3.3. Let $Y_N^{(s-1)}$ be the sample set generated by Algorithm 3.3.2. Then we have*

$$D_{N,\psi}^*(Y_N^{(s-1)}) \leq \sum_{j=1}^{k-1} \frac{C_{\mathcal{S}_\ell, \psi_{k-\ell+1}} \alpha_j^{1-1/s} \log(\alpha_\ell N)}{N^{1/s}} + \sum_{\ell=1}^{k} \frac{C_{\mathcal{L}_\ell, H_\ell} (\log \beta_\ell N)^{s-1}}{N} + \frac{1}{N},$$

where

$$\alpha_\ell = \frac{\int_{\mathcal{S}_\ell} \psi_{k-\ell+1}(\boldsymbol{x})d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x})d\boldsymbol{x}} \quad \text{and} \quad \beta_\ell = \frac{\int_{\mathcal{L}_\ell} H_\ell(\boldsymbol{x})d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x})d\boldsymbol{x}},$$

and $C_{\mathcal{S}_\ell,\psi_{k-\ell+1}}$ and $C_{\mathcal{L}_\ell,H_\ell}$ are constants depending on $\mathcal{S}_\ell, \psi_{k-\ell+1}$ and $\mathcal{L}_\ell, H_\ell$ respectively.

3.4 A δ-cover to approximation of the star-discrepancy

Since it is computationally too expensive to compute the supremum in the definition of the star-discrepancy exactly for dimensions larger than one, we use a so-called δ-cover to estimate this supremum.

Definition 3.4.1. *Let $(G, \mathcal{B}(G), \psi)$ be a probability space where $G \subseteq \mathbb{R}^{s-1}$ and $\mathcal{B}(G)$ is the Borel σ-algebra defined on G. Let $\mathscr{A} \subseteq \mathcal{B}(G)$ be a set of test sets. A finite subset $\Gamma_\delta \subseteq \mathscr{A}$ is called a δ-cover of $\mathscr{A}$ with respect to ψ if for every $A \in \mathscr{A}$ there are sets $C, D \in \Gamma_\delta$ such that*

$$C \subseteq A \subseteq D$$

and

$$\psi(D \setminus C) \leq \delta.$$

The concept of δ-cover is motivated by the following result from [26, Lemma 3.1] and [38, Section 2.1]. Assume that Γ_δ is a δ-cover of $\mathscr{A}$ with respect to the distribution ψ. For all $\{\boldsymbol{z}_0, \boldsymbol{z}_1, \ldots, \boldsymbol{z}_{N-1}\}$, the following discrepancy inequality holds

$$\sup_{A\in\mathscr{A}} \left| \frac{1}{N} \sum_{n=0}^{N-1} 1_{\boldsymbol{z}_n \in A} - \psi(A) \right| \leq \max_{C\in\Gamma_\delta} \left| \frac{1}{N} \sum_{n=0}^{N-1} 1_{\boldsymbol{z}_n \in C} - \psi(C) \right| + \delta.$$

It can be verified as follows: Since Γ_δ is a δ-cover of $\mathscr{A}$ with respect to ψ, for any $A \in \mathscr{A}$, there are sets $C, D \in \Gamma_\delta$ such that $C \subseteq A \subseteq D$ and $\psi(D \setminus C) \leq \delta$. Then we have

$$\frac{1}{N} \sum_{n=0}^{N-1} 1_{\boldsymbol{z}_n \in C} - \psi(C) - \delta \leq \frac{1}{N} \sum_{n=0}^{N-1} 1_{\boldsymbol{z}_n \in A} - \psi(A) \leq \frac{1}{N} \sum_{n=0}^{N-1} 1_{\boldsymbol{z}_n \in D} - \psi(D) + \delta.$$

The desired result follows by taking the absolute value of the middle term in the above formula. In the experiments we choose $\mathscr{A}$ to be the set of intervals $[\boldsymbol{0}, \boldsymbol{t})$,

where $\boldsymbol{t}$ runs through all points in the domain. For densities defined in $[0,1]^{s-1}$, we set

$$\Gamma_\delta = \left\{ \prod_{j=1}^{s-1} [0, a_j 2^{-m}) : a_j \in \mathbb{Z}, 0 \leq a_j \leq 2^m \right\},$$

which means that the δ-cover becomes finer as the number of samples increases, thus it can yield a more accurate approximation of the star-discrepancy.

For densities defined in $\mathbb{R}^{s-1}$, we choose δ-covers with respect to m as

$$\Gamma_\delta = \left\{ \prod_{j=1}^{s-1} (0, F_j^{-1}(a_j 2^{-m})) : a_j \in \mathbb{Z}, 0 \leq a_j \leq 2^m \right\},$$

where F_j^{-1} is the inverse marginal CDF with respect to the proposal density H. Note that the approximation of the star-discrepancy is computationally expensive, thus our experiments only go up to several thousand sample points. However, the generation of samples using a (t, m, s)-net is fast.

3.5 Numerical experiments

In the following we present some numerical results. Since in general it is computationally too expensive to compute the supremum in the definition of the star-discrepancy exactly, we use a so-called δ-cover to estimate this supremum.

In the numerical discussion, the driver sequence is generated by a (t, m, s)-net in base 2. Specifically, we always use a Sobol′ sequence [77] to generate (t, m, s)-nets for our experiments. We consider now the case where the target density is defined on $[0,1]^{s-1}$. The following test is a deterministic version of Algorithm 2.4.1. For the proofs later, we need the technical assumption that the target density is pseudo-convex.

The following example shows a better convergence rate when using a low-discrepancy driver sequence rather than a random point set. The reported discrepancy for the acceptance-rejection algorithm using a random driver sequence in this section is the average of 10 independent runs. Note that numerical results in figures are presented in a log-log scale, which is throughout the thesis.

Example 3.5.1. *In this example we consider a non-product target density in* $[0,1]^4$. *Let the target density* ψ *be*

$$\psi(x_1,x_2,x_3,x_4) = \frac{1}{4}(e^{-x_1}+e^{-x_2}+e^{-x_3}+e^{-x_4}), \quad (x_1,x_2,x_3,x_4) \in [0,1]^4.$$

Figure 3.7 shows the discrepancy by using deterministic points and pseudo-random points as driver sequence. For the plain acceptance-rejection algorithm, we observe a convergence rate of $N^{-0.482}$, whereas the deterministic acceptance-rejection algorithm using (t,m,s)-nets based on a Sobol′ sequence shows a convergence rate of the discrepancy of order $N^{-0.659}$.

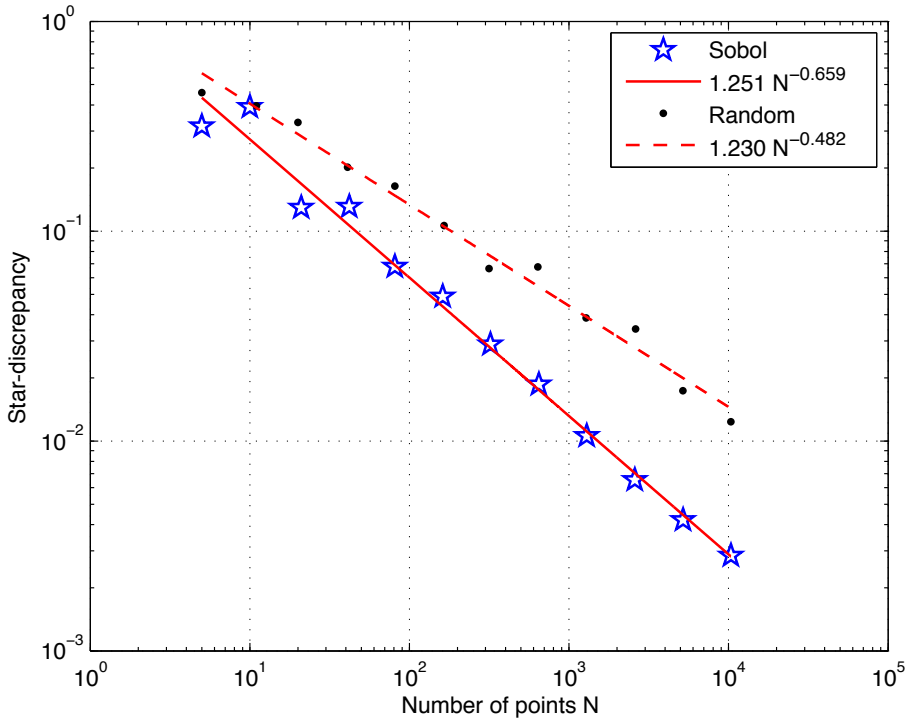


Figure 3.7: Convergence order of the star-discrepancy of Example 3.5.1 for a target density defined in cube.

Next we provide an example to demonstrate the performance of Algorithm 3.2.6 for a target density with state space defined over the real numbers.

Example 3.5.2. *Let the target density function be given by*

$$\psi(x_1, x_2) = \begin{cases} \frac{4}{\pi} e^{-(x_1+x_2)} (x_1 x_2)^{1/2}, & x_1, x_2 > 0, \\ 0, & \textit{else.} \end{cases}$$

The proposal density function H, which we use to do the acceptance-rejection to generate samples of $\psi(x_1, x_2)$, is chosen as

$$H(x_1, x_2) = \begin{cases} \frac{1}{4}, & 0 \le x_1, x_2 \le 1, \\ \frac{1}{4x_2^2}, & 0 \le x_1 \le 1, x_2 > 1, \\ \frac{1}{4x_1^2}, & x_1 > 1, 0 \le x_2 \le 1, \\ \frac{1}{4x_1^2 x_2^2}, & x_1, x_2 > 1, \\ 0, & \text{else.} \end{cases}$$

For this choice of H, we use the transform T defined in Equation (3.2.2) to obtain samples from H. The samples $(x_{j,1}, x_{j,2})$ are given by the following transformation

$$x_{j,1} = \begin{cases} 2u_{j,1}, & 0 \le u_{j,1} \le 1/2, \\ 1/2(1 - u_{j,1}), & 1/2 < u_{j,1} \le 1, \end{cases}$$

$$x_{j,2} = \begin{cases} 2u_{j,2}, & 0 \le u_{j,2} \le 1/2, \\ 1/2(1 - u_{j,2}), & 1/2 < u_{j,2} \le 1, \end{cases}$$

where $(u_{j,1}, u_{j,2}), 0 \le j \le b^m$, is the driver point set given by a $(t, m, 2)$-net in base b.

The order of convergence of the star-discrepancy is demonstrated in Figure 3.8, where N is the number of accepted samples. The numerical experiments show that the star-discrepancy converges at a rate of $N^{-0.720}$ for this example using quasi-Monte Carlo samples as proposal. The original acceptance-rejection algorithm converges with order $N^{-0.464}$. Again, the deterministic version sampler outperforms the pseudo-random sampler.

Now we present an example for sampling from a target density function using the reduced acceptance-rejection sampler.

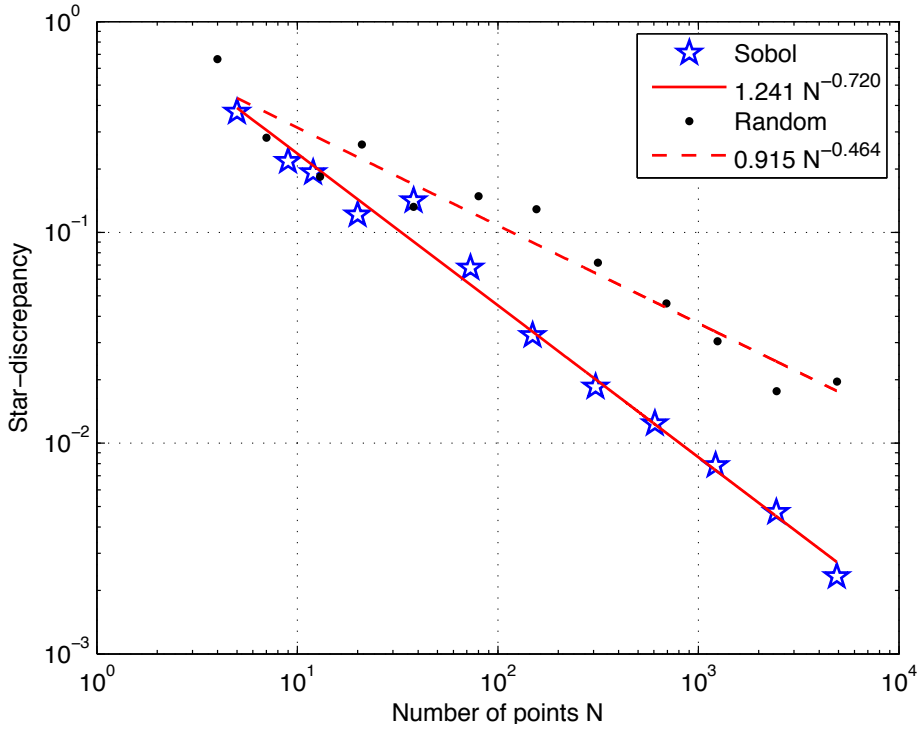


Figure 3.8: Convergence order of the star-discrepancy of Example 3.5.2 for a target density defined in real state space.

Example 3.5.3. *Let* $\psi(x) = \sin(4x) + x^2$ *be the target density function defined on* $[0, 1]$.

Instead of seeking a proposal density H such that $\psi(x) \leq H(x)$, we notice that inversion can be implied to $\sin(4x)$ and x^2 independently. However, it can not work for their sum. Choose $H(x) = x^2$. We only do deterministic acceptance-rejection with respect to the target density ψ and proposal density H in the subinterval $\mathcal{S} = (\pi/4, 1]$. In the remaining range $\mathcal{L} = [0, \pi/4]$, we apply the inverse transformation on H and $\psi - H$ to obtain samples based on a deterministic driver sequence.

The discrepancy of the point set generated by Algorithm 3.3.1 converges at the rate of $N^{-0.929}$, which is significantly better than the $N^{-0.501}$ convergence rate of a random driver sequence, see Figure 3.9.

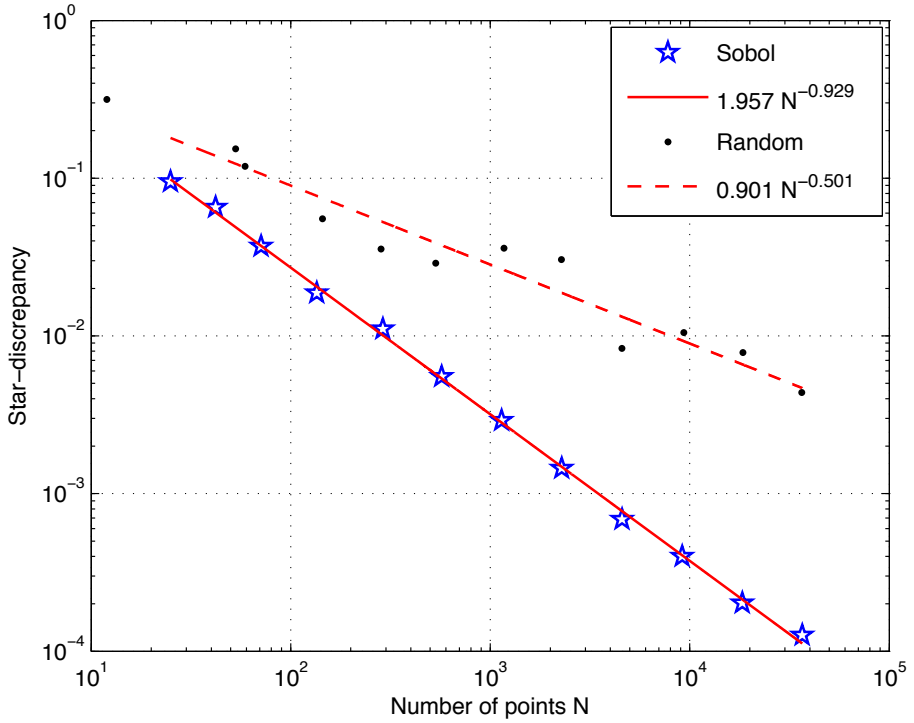


Figure 3.9: Convergence order of the star-discrepancy of Example 3.5.3 using the reduced deterministic acceptance-rejection sampler.

3.6 Proofs

Before giving the proofs, we need some preparation.

Consider the following elementary intervals

$$W_k = \prod_{j=1}^{s} \left[\frac{c_j}{b^k}, \frac{c_j + 1}{b^k} \right), \tag{3.6.1}$$

with $0 \leq c_j < b^k$ (where c_j is an integer) for $j = 1, \ldots, s$. The diagonal of W_k has length $\sqrt{s}/b^k$ and the volume is b^{-sk}. Let J be an arbitrary convex set in $[0,1]^s$. Let W_k^o denote the union of cubes W_k fully contained in J,

$$W_k^o = \bigcup_{W_k \subseteq J} W_k. \tag{3.6.2}$$

Let $\overline{W}_k$ denote the union of cubes W_k having non-empty intersection with J or its boundary $\partial(J)$,

$$\overline{W}_k = \bigcup_{W_k \cap (J \cup \partial(J)) \neq \emptyset} W_k. \tag{3.6.3}$$

Lemma 3.6.1. *Let $k \in \mathbb{N}$. Let J be an arbitrary convex set in $[0,1]^s$. For the W_k^o and $\overline{W}_k$ constructed by (3.6.2) and (3.6.3), we have*

$$\lambda(\overline{W}_k \setminus J) \leq 2sb^{-k} \text{ and } \lambda(J \setminus W_k^o) \leq 2sb^{-k}.$$

To illustrate the result we provide the following simple argument which yields a slightly weaker result. Since the diagonal of W_k has length $\sqrt{s}/b^k$ we have

$$\overline{W}_k \setminus J \subseteq B := \{\boldsymbol{x} \in [0,1]^s \setminus J : \|\boldsymbol{x} - \boldsymbol{y}\| \leq \sqrt{s}b^{-k} \text{ for some } \boldsymbol{y} \in J\},$$

where $\|\cdot\|$ is the Euclidean norm. Then

$$\lambda(\overline{W}_k \setminus J) \leq \lambda(B).$$

Note that the outer surface area of a convex set in $[0,1]^s$ is bounded by the surface area of the unit cube $[0,1]^s$, which is $2s$. Thus the Lebesgue measure of the set B is bounded by the outer surface area times the diameter. Therefore

$$\lambda(\overline{W}_k \setminus J) \leq \lambda(B) \leq 2s\sqrt{s}b^{-k}.$$

The result for $\lambda(J \setminus W_k^o)$ follows by a similar discussion as the proof above.

Remark. *Note that in [61] it was also shown that the constant $2s$ is best possible.*

Now we extend the result in Lemma 3.6.1 to pseudo-convex sets.

Corollary 3.6.2. *Let J be an arbitrary pseudo-convex set in $[0,1]^s$ with admissible convex covering of p parts with q convex parts of J. For W_k^o and $\overline{W}_k$ given by (3.6.2) and (3.6.3) we have*

$$\lambda(\overline{W}_k \setminus J) \leq 2psb^{-k} \text{ and } \lambda(J \setminus W_k^o) \leq 2psb^{-k}.$$

Proof. Let $A_1, \ldots, A_p$ be an admissible convex covering of J with p parts. Without loss of generality, let $A_1, \ldots, A_q$ be the convex subsets of J and $A_{q+1}, \ldots, A_p$ be such that $A_j' = A_j \setminus J$ is convex for $q+1 \leq j \leq p$. It follows that

$$J = \bigcup_{j=1}^{q} A_j \cup \bigcup_{j=q+1}^{p} (A_j \setminus A_j'). \tag{3.6.4}$$

Therefore

$$\overline{W}_k \setminus J \subseteq \left(\bigcup_{j=1}^{q} B_j \cup \bigcup_{j=q+1}^{p} B'_j \right),$$

where

$$B_j = \left\{ \boldsymbol{y} \in [0,1]^s \setminus A_j : \|\boldsymbol{x} - \boldsymbol{y}\| \leq \sqrt{s} b^{-k} \text{ for some } \boldsymbol{x} \in A_j \right\}, \ j = 1, \ldots, q,$$

and

$$B'_j = \{ \boldsymbol{y} \in A'_j : \|\boldsymbol{x} - \boldsymbol{y}\| \leq \sqrt{s} b^{-k} \text{ for some } \boldsymbol{x} \in [0,1]^s \setminus A'_j \}, \ j = q+1, \ldots, p.$$

Since $B_j \cup A_j$ for $j = 1, \ldots, q$, and $B'_j \cup A'_j$ for $j = q+1, \ldots, p$ are convex, using Lemma 3.6.1, we obtain

$$\lambda(\overline{W}_k \setminus J) \leq \lambda\Big(\bigcup_{j=1}^{q} B_j \Big) + \lambda\Big(\bigcup_{j=q+1}^{p} B'_j \Big) \leq 2psb^{-k}.$$

The result for $\lambda(J \setminus W_k^o)$ follows by a similar discussion. □

Proof of Lemma 3.1.7. For the point set $Q_{m,s} = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{M-1}\} \subseteq [0,1]^s$ generated by a (t, m, s)-net in base b with $M = b^m$, let $k = \left\lfloor \frac{m-t}{s} \right\rfloor$. Let J be an arbitrary convex set in $[0,1]^s$. Consider the elementary interval W_k given by Equation (3.6.1). For W_k^o and $\overline{W}_k$ given by (3.6.2) and (3.6.3), obviously, $W_k^o \subseteq J \subseteq \overline{W}_k$. The sets W_k^o and $\overline{W}_k$ are fair with respect to the net, that is

$$\frac{1}{M} \sum_{n=0}^{M-1} 1_{\overline{W}_k}(\boldsymbol{x}_n) = \lambda(\overline{W}_k) \quad \text{and} \quad \frac{1}{M} \sum_{n=0}^{M-1} 1_{W_k^o}(\boldsymbol{x}_n) = \lambda(W_k^o).$$

Then

$$\begin{aligned} \frac{1}{M} \sum_{n=0}^{M-1} 1_J(\boldsymbol{x}_n) - \lambda(J) \leq & \frac{1}{M} \sum_{n=0}^{M-1} 1_{\overline{W}_k}(\boldsymbol{x}_n) - \lambda(\overline{W}_k) + \lambda(\overline{W}_k \setminus J) \\ = & \lambda(\overline{W}_k \setminus J), \end{aligned}$$

and

$$\begin{aligned} \frac{1}{M} \sum_{n=0}^{M-1} 1_J(\boldsymbol{x}_n) - \lambda(J) \geq & \frac{1}{M} \sum_{n=0}^{M-1} 1_{W_k^o}(\boldsymbol{x}_n) - \lambda(W_k^o) - \lambda(J \setminus W_k^o) \\ = & -\lambda(J \setminus W_k^o). \end{aligned}$$

By Lemma 3.6.1, we have

$$\lambda(\overline{W}_k \setminus J) \le 2sb^{-k} \text{ and } \lambda(J \setminus W_k^o) \le 2sb^{-k}.$$

Thus we obtain

$$\left| \frac{1}{M} \sum_{n=0}^{M-1} 1_J(\boldsymbol{x}_n) - \lambda(J) \right| \le 2sb^{-k} \le 2sb^{t/s} M^{-1/s}.$$

Since the bound holds for arbitrary convex sets, the proof is completed. □

3.6.1 Proof of Theorem 3.2.3

Now we are ready to prove the upper bound.

Proof of Theorem 3.2.3. Let $J_{\boldsymbol{t}}^* = ([\boldsymbol{0}, \boldsymbol{t}) \times [0,1]) \bigcap A$, where $\boldsymbol{t} = (t_1, \dots, t_{s-1})$ and $A = \{\boldsymbol{x} \in [0,1]^s : \psi(x_1, , \dots, x_{s-1}) \ge Lx_s\}$. Since $\boldsymbol{y}_n$ consists of the first $s-1$ coordinates of $\boldsymbol{z}_n \in A$ for $n = 0, \dots, N-1$, we have

$$\sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) = \sum_{n=0}^{N-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{z}_n) = \sum_{n=0}^{N-1} 1_{[\boldsymbol{0},\boldsymbol{t})}(\boldsymbol{y}_n).$$

Therefore

$$\left| \frac{1}{N} \sum_{n=0}^{N-1} 1_{[\boldsymbol{0},\boldsymbol{t})}(\boldsymbol{y}_n) - \frac{1}{C} \int_{[\boldsymbol{0},\boldsymbol{t})} \psi(\boldsymbol{z}) d\boldsymbol{z} \right| = \left| \frac{1}{N} \sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) - \frac{1}{\lambda(A)} \lambda(J_{\boldsymbol{t}}^*) \right|.$$

The right-hand side above is now bounded by

$$\begin{aligned} & \frac{M}{N} \left| \frac{1}{M} \sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) - \lambda(J_{\boldsymbol{t}}^*) \right| + \left| \lambda(J_{\boldsymbol{t}}^*) \left(\frac{M}{N} - \frac{1}{\lambda(A)} \right) \right| \\ \le \; & \frac{M}{N} \left(\left| \frac{1}{M} \sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) - \lambda(J_{\boldsymbol{t}}^*) \right| + \left| \lambda(A) - \frac{1}{M} \sum_{n=0}^{M-1} 1_A(\boldsymbol{x}_n) \right| \right), \end{aligned}$$

where we used the estimation $\lambda(J_{\boldsymbol{t}}^*) \le \lambda(A)$ and the fact that $N = \sum_{n=0}^{M-1} 1_A(\boldsymbol{x}_n)$. Since $J_{\boldsymbol{t}}^*$ is also pseudo-convex, it follows from Lemma 3.1.9 that we can bound the above expression by

$$\frac{M}{N} 2(2p-q) J_M(P_M^{(s)}).$$

In addition, $\lim_{M\to\infty} \frac{N}{M} = \lambda(A)$, which means $\lim_{M\to\infty} \frac{N}{M} = \int_{[0,1]^{s-1}} \psi(\boldsymbol{z})d\boldsymbol{z}/L = C/L$. Hence there is an M_0 such that $\frac{N}{M} \geq C/(2L)$ for all $M \geq M_0$. Thus $\frac{M}{N} \leq \frac{2L}{C}$ for all $M \geq M_0$. Further we have $N \leq M$. Using Lemma 3.1.7 we obtain the bound

$$\frac{M}{N} 2(2p-q)J_M(P_M^{(s)}) \leq 8LC^{-1}sb^{t/s}(2p-q)N^{-1/s}.$$

□

3.6.2 Proof of Theorem 3.2.4

The following lemma provides information about the packing number of the northern hemisphere

$$\mathbb{S}^{s-1}_{\text{north}} := \{\boldsymbol{x} \in [0,1]^s, \|\boldsymbol{x} - \mathbf{1/2}\| = 1/2, x_s \geq 0\},$$

where $\mathbf{1/2} = (\frac{1}{2}, \frac{1}{2}, \ldots, \frac{1}{2}) \in [0,1]^s$. The (closed) spherical cap $C(\boldsymbol{y}, \rho) \subseteq \mathbb{S}^{s-1}_{\text{north}}$ with center $\boldsymbol{y} \in \mathbb{S}^{s-1}_{\text{north}}$ and angular radius $\rho \in [0, \pi]$ is defined by

$$C(\boldsymbol{y}, \rho) = \{\boldsymbol{y} \in \mathbb{S}^{s-1}_{\text{north}} | \boldsymbol{x} \cdot \boldsymbol{y} \geq \frac{\cos\rho}{4}\}.$$

The packing of $\mathbb{S}^{s-1}_{\text{north}}$ considered here is constructed by identical spherical caps which are non-overlapping, that is, $C(\boldsymbol{y}_i, \rho)$ and $C(\boldsymbol{y}_j, \rho)$ with $i \neq j$ touch at most at their boundaries.

Lemma 3.6.3. *Let $s \geq 1$. For any $n \in \mathbb{N}$ there exist M_n points $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_{M_n}$ on the northern hemisphere $\mathbb{S}^s_{north} \subseteq [0,1]^{s+1}$ and an angular radius ρ_n, with*

$$\rho_n = c_1(2n)^{-1/(s-1)},$$
$$n \leq M_n \leq c_2 n,$$

such that the caps $C(\boldsymbol{y}_i, \rho_n)$, $i = 1, \ldots, M_n$, form a packing of the northern hemisphere. The positive constants c_1, c_2 depend only on the dimension s.

The lemma is essentially well-known for spheres. The explicit proof is due to Wyner [86] and Hesse gives a summary in [39, Lemma 1]. A similar argument can be used for the hemisphere in our case.

Now we give the proof of Theorem 3.2.4 whose proof follows the argument from the proof of [73, Theorem 1].

Proof. We may suppose that $s \geq 2$. Let $\mathbb{S}^{s-1}_{\text{north}}$ be the northern hemisphere defined above contained in $[0,1]^s$, and let S be the surface of $\mathbb{S}^{s-1}_{\text{north}}$. Let C be a closed spherical cap on S with spherical radius ρ. The convex hull $\overline{C}$ of C is a solid spherical cap. For $0 < \rho < \pi/2$, $\lambda(\overline{C})$ is a continuous function of ρ with

$$c_1\rho^{s+1} < \lambda(\overline{C}) < c_2\rho^{s+1}. \tag{3.6.5}$$

If N is sufficiently large, there is a positive real number ρ_0 such that a cap C of spherical radius ρ_0 has

$$\lambda(\overline{C}) = \frac{1}{2N}.$$

In view of (3.6.5), $0 < \rho_0 < c_3 N^{-1/(s+1)}$. We now pick as many pairwise disjoint caps with radius ρ_0 as possible, say $C_1, \ldots, C_M$. By Lemma 3.6.3, for large N and hence small ρ_0 we have $M \geq c_4\rho_0^{-(s-1)}$, hence

$$M \geq c_5 N^{(s-1)/(s+1)}. \tag{3.6.6}$$

Given a sequence of numbers $\sigma_1, \ldots, \sigma_M$, with each σ_i either 1 or -1, let $B(\sigma_1, \ldots, \sigma_M)$ consist of all $x \in \mathbb{S}^{s-1}_{\text{north}}$ which do not lie in a cap $\overline{C_i}$ with $\sigma_i = -1$. In other words, $B(\sigma_1, \ldots, \sigma_M)$ is obtained from $\mathbb{S}^{s-1}_{\text{north}}$ by removing the solid caps $\overline{C_i}$ for which $\sigma_i = -1$.

Now the local discrepancy function $\Delta_{P_N}(H)$ defined by

$$\Delta_{P_N}(H) = \sum_{i=1}^{N} 1_H(P_N) - N\lambda(H)$$

is additive, i.e. it satisfies

$$\Delta_{P_N}(H \cup H') = \Delta_{P_N}(H) + \Delta_{P_N}(H')$$

if $H \cap H' = \emptyset$. It follows easily that

$$\Delta_{P_N}(B(\sigma_1, \ldots, \sigma_M)) - \Delta_{P_N}(B(-\sigma_1, \ldots, -\sigma_M)) = \sum_{i=1}^{M} \sigma_i \Delta_{P_N}(\overline{C_i}).$$

We have

$$\Delta_{P_N}(\overline{C_i}) = \sum_{i=1}^{N} 1_{\overline{C_i}}(P_N) - N\lambda(\overline{C_i}) = \sum_{i=1}^{N} 1_{\overline{C_i}}(P_N) - \frac{1}{2}.$$

Hence for every i, either $\Delta_{P_N}(\overline{C_i}) \geq \frac{1}{2}$ or $\Delta_{P_N}(\overline{C_i}) = -\frac{1}{2}$. Choose σ_i such that $\sigma_i \Delta_{P_N}(\overline{C_i}) \geq 1/2$ for $1 \leq i \leq M$. Then

$$\Delta_{P_N}(B(\sigma_1, \ldots, \sigma_M)) - \Delta_{P_N}(B(-\sigma_1, \ldots, -\sigma_M)) \geq M/2,$$

and either $J = B(\sigma_1, \ldots, \sigma_M)$ or $J = B(-\sigma_1, \ldots, -\sigma_M)$ has $|\Delta_{P_N}(J)| \geq M/4$. In addition, J is a convex set due to its construction.

Thus by (3.6.6),

$$D_N^*(\lambda, J) \geq \frac{1}{4}\frac{M}{N} \geq c_6 N^{-2/(s+1)}.$$

We take ψ as the boundary of J excluding the boundary of $[0,1]^s$, which completes the proof. □

3.6.3 Proof of Lemma 3.2.10

Now we prove Lemma 3.2.10 which plays an important role for obtaining the improved upper bound.

Proof of Lemma 3.2.10. Let $\boldsymbol{t} \in [0,1]^s$ be given. Let $v = \Gamma_{m-t}(\psi)$ and $U_1, \ldots, U_v$ be elementary intervals of order $m-t$ such that $U_1 \cup U_2 \cup \cdots \cup U_v \supseteq (\partial J_{\boldsymbol{t}}^* \setminus \partial[0,1]^s)$ and $U_i \cap U_{i'} = \emptyset$ for $1 \leq i < i' \leq v$. Let $V_1, \ldots, V_z \in \mathcal{E}_{m-t}$ with $V_i \subseteq J_{\boldsymbol{t}}^*$, $V_i \cap V_{i'} = \emptyset$ for all $1 \leq i < i' \leq z$ and $V_i \cap U_i = \emptyset$ such that $J_{\boldsymbol{t}}^* \subseteq \bigcup_{i=1}^z V_i \cup \bigcup_{i=1}^v U_i$. We define

$$\overline{W} = \bigcup_{i=1}^{z} V_i \cup \bigcup_{i=1}^{v} U_i$$

and

$$W^o = \bigcup_{i=1}^{z} V_i.$$

Then $\overline{W}$ and W^o are fair with respect to the (t, m, s)-net, $W^o \subseteq J_{\boldsymbol{t}}^* \subseteq \overline{W}$ and

$$\lambda(\overline{W} \setminus J_{\boldsymbol{t}}^*), \lambda(J_{\boldsymbol{t}}^* \setminus W^o) \leq \lambda(\overline{W} \setminus W^o) = \sum_{i=1}^{v} \lambda(U_i) = \sum_{i=1}^{v} b^{-m+t} = b^{-m+t}\Gamma_{m-t}(\psi).$$

The proof of the desired result now follows by the same arguments as the proof of Theorem 3.2.3 as presented in Section 3.6.1.

□

3.6.4 Proof of Theorem 3.3.3

Now we give the proof of the upper bound on the discrepancy for samples generated by the reduced acceptance-rejection sampler associated with one special class of density function. In what follows we restrict our investigations to the case $k = 2$ for simplicity, the general case can be proved by similar arguments.

Proof. Let $\psi = H_1 + H_2$ be the target density function. Assume that we can apply the inverse CDF on H_1 and H_2 to generate samples. Let

$$\mathcal{S} := \{\boldsymbol{x} \in D \subseteq \mathbb{R}^{s-1} : \psi(\boldsymbol{x}) < H_1(\boldsymbol{x})\},$$

and

$$\mathcal{L} := \{\boldsymbol{x} \in D \subseteq \mathbb{R}^{s-1} : \psi(\boldsymbol{x}) \geq H_1(\boldsymbol{x})\}.$$

The final sample set $Y_N^{(s-1)}$ is a superposition of the three subsets, $Y_{1,1}^{(s-1)}, Y_{1,2}^{(s-1)}$ and $Y_{2,2}^{(s-1)}$, see Figure 3.6. Define $Y_{i,\ell}^{(s-1)} = \{x_0^{(i,\ell)}, x_1^{(i,\ell)}, \ldots, x_{N_{i,\ell}-1}^{(i,\ell)}\}$ for $i, \ell = 1, 2$. The number $N_{i,\ell}$ of the points in each subset is given by

$$\begin{aligned} N_{1,1} &= \left\lceil N \frac{\int_{\mathcal{S}} \psi(\boldsymbol{x}) d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x}) d\boldsymbol{x}} \right\rceil, \\ N_{1,2} &= \left\lceil N \frac{\int_{\mathcal{L}} H_1(\boldsymbol{x}) d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x}) d\boldsymbol{x}} \right\rceil, \\ N_{2,2} &= \left\lceil N \frac{\int_{\mathcal{L}} H_2(\boldsymbol{x}) d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x}) d\boldsymbol{x}} \right\rceil. \end{aligned}$$

Then there exists $\delta_i \in [0, 1)$ for $i = 1, 2, 3$ such that

$$\begin{aligned} N_{1,1} &= N \frac{\int_{\mathcal{S}} \psi(\boldsymbol{x}) d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x}) d\boldsymbol{x}} + \delta_1, \\ N_{1,2} &= N \frac{\int_{\mathcal{L}} H_1(\boldsymbol{x}) d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x}) d\boldsymbol{x}} + \delta_2, \\ N_{2,2} &= N \frac{\int_{\mathcal{L}} H_2(\boldsymbol{x}) d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x}) d\boldsymbol{x}} + \delta_3. \end{aligned}$$

Therefore, we have

$$
\begin{aligned}
&\left|\frac{1}{N}\sum_{n=0}^{N-1} 1_{(-\infty,\boldsymbol{t}]\cap D}(\boldsymbol{x}_n) - \frac{\int_{(-\infty,\boldsymbol{t}]\cap D}\psi(\boldsymbol{x})d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x})d\boldsymbol{x}}\right| \\
=&\left|\frac{1}{N}\sum_{n=0}^{N-1} 1_{(-\infty,\boldsymbol{t}]\cap D}(\boldsymbol{x}_n) - \frac{\int_{(-\infty,\boldsymbol{t}]\cap\mathcal{L}} H_1(\boldsymbol{x})d\boldsymbol{x} + \int_{(-\infty,\boldsymbol{t}]\cap\mathcal{L}} H_2(\boldsymbol{x})d\boldsymbol{x} + \int_{(-\infty,\boldsymbol{t}]\cap\mathcal{S}}\psi(\boldsymbol{x})d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x})d\boldsymbol{x}}\right| \\
\le&\left|\frac{1}{N}\sum_{n=0}^{N_{1,1}-1} 1_{(-\infty,\boldsymbol{t}]\cap D}(\boldsymbol{x}_n^{(1,1)}) - \frac{\int_{(-\infty,\boldsymbol{t}]\cap\mathcal{L}} H_1(\boldsymbol{x})d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x})d\boldsymbol{x}}\right| \\
+&\left|\frac{1}{N}\sum_{n=0}^{N_{1,2}-1} 1_{(-\infty,\boldsymbol{t}]\cap D}(\boldsymbol{x}_n^{(1,2)}) - \frac{\int_{(-\infty,\boldsymbol{t}]\cap\mathcal{L}} H_2(\boldsymbol{x})d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x})d\boldsymbol{x}}\right| \\
+&\left|\frac{1}{N}\sum_{n=0}^{N_{2,2}-1} 1_{(-\infty,\boldsymbol{t}]\cap D}(\boldsymbol{x}_n^{(2,2)}) - \frac{\int_{(-\infty,\boldsymbol{t}]\cap\mathcal{S}}\psi(\boldsymbol{x})d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x})d\boldsymbol{x}}\right| \\
=&\frac{N_{1,1}}{N}\left|\frac{1}{N_{1,1}}\sum_{n=0}^{N_{1,1}-1} 1_{(-\infty,\boldsymbol{t}]\cap D}(\boldsymbol{x}_n^{(1,1)}) - \frac{N}{N_{1,1}}\frac{\int_{(-\infty,\boldsymbol{t}]\cap\mathcal{S}}\psi(\boldsymbol{x})d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x})d\boldsymbol{x}}\right| \\
+&\frac{N_{1,2}}{N}\left|\frac{1}{N_{1,2}}\sum_{n=0}^{N_{1,2}-1} 1_{(-\infty,\boldsymbol{t}]\cap D}(\boldsymbol{x}_n^{(1,2)}) - \frac{N}{N_{1,2}}\frac{\int_{(-\infty,\boldsymbol{t}]\cap\mathcal{L}} H_1(\boldsymbol{x})d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x})d\boldsymbol{x}}\right| \\
+&\frac{N_{2,2}}{N}\left|\frac{1}{N_{2,2}}\sum_{n=0}^{N_{2,2}-1} 1_{(-\infty,\boldsymbol{t}]\cap D}(\boldsymbol{x}_n^{(2,2)}) - \frac{N}{N_{2,2}}\frac{\int_{(-\infty,\boldsymbol{t}]\cap\mathcal{L}} H_2(\boldsymbol{x})d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x})d\boldsymbol{x}}\right| \\
:=&I_1 + I_2 + I_3.
\end{aligned}
$$

Since

$$
\begin{aligned}
I_1 =&\frac{N_{1,1}}{N}\left[\left|\frac{1}{N_{1,1}}\sum_{n=0}^{N_{1,1}-1} 1_{(-\infty,\boldsymbol{t}]\cap D}(\boldsymbol{x}_n^{(1,1)}) - \frac{\int_{(-\infty,\boldsymbol{t}]\cap\mathcal{S}}\psi(\boldsymbol{x})d\boldsymbol{x}}{\int_{\mathcal{S}}\psi(\boldsymbol{x})d\boldsymbol{x}}\right| + \frac{\delta_1}{N_{1,1}}\frac{\int_{(-\infty,\boldsymbol{t}]\cap\mathcal{S}}\psi(\boldsymbol{x})d\boldsymbol{x}}{\int_{\mathcal{S}}\psi(\boldsymbol{x})d\boldsymbol{x}}\right], \\
I_2 =&\frac{N_{1,2}}{N}\left[\left|\frac{1}{N_2}\sum_{n=0}^{N_{1,2}-1} 1_{(-\infty,\boldsymbol{t}]\cap D}(\boldsymbol{x}_n^{(1,2)}) - \frac{\int_{(-\infty,\boldsymbol{t}]\cap\mathcal{L}} H_1(\boldsymbol{x})d\boldsymbol{x}}{\int_{\mathcal{L}} H_1(\boldsymbol{x})d\boldsymbol{x}}\right| + \frac{\delta_2}{N_{1,2}}\frac{\int_{(-\infty,\boldsymbol{t}]\cap\mathcal{L}} H_1(\boldsymbol{x})d\boldsymbol{x}}{\int_{\mathcal{L}} H_1(\boldsymbol{x})d\boldsymbol{x}}\right], \\
I_3 =&\frac{N_{2,2}}{N}\left[\left|\frac{1}{N_{2,2}}\sum_{n=0}^{N_{2,2}-1} 1_{(-\infty,\boldsymbol{t}]\cap D}(\boldsymbol{x}_n^{(2,2)}) - \frac{\int_{(-\infty,\boldsymbol{t}]\cap\mathcal{L}} H_2(\boldsymbol{x})d\boldsymbol{x}}{\int_{\mathcal{L}} H_2(\boldsymbol{x})d\boldsymbol{x}}\right| + \frac{\delta_3}{N_{2,2}}\frac{\int_{(-\infty,\boldsymbol{t}]\cap\mathcal{L}} H_2(\boldsymbol{x})d\boldsymbol{x}}{\int_{\mathcal{L}} H_2(\boldsymbol{x})d\boldsymbol{x}}\right],
\end{aligned}
$$

then we obtain

$$
\begin{aligned}
&I_1 + I_2 + I_3 \\
\leq &\frac{N_{1,1}}{N} D^*_{\mathcal{S},\psi}(Y^{(s-1)}_{1,1}) + \frac{N_{1,2}}{N} D^*_{\mathcal{L},H_1}(Y^{(s-1)}_{1,2}) + \frac{N_{2,2}}{N} D^*_{\mathcal{L},H_2}(Y^{(s-1)}_{2,2}) + \frac{1}{N} \frac{\int_{(-\infty,\boldsymbol{t}]\cap D} \psi(\boldsymbol{x}) d\boldsymbol{x}}{\int_D \psi(\boldsymbol{x}) d\boldsymbol{x}} \\
\leq &\frac{N_{1,1}}{N} D^*_{\mathcal{S},\psi}(Y^{(s-1)}_{1,1}) + \frac{N_{1,2}}{N} D^*_{\mathcal{L},H_1}(Y^{(s-1)}_{1,2}) + \frac{N_{2,2}}{N} D^*_{\mathcal{L},H_2}(Y^{(s-1)}_{2,2}) + \frac{1}{N},
\end{aligned}
$$

where $D^*_{\mathcal{S},\psi}$ is the star-discrepancy of sample points in $\mathcal{S}$ associated with ψ and the same notation is also applied to $D^*_{\mathcal{L},H_1}$ and $D^*_{\mathcal{L},H_2}$.

Since this result holds for arbitrary $\boldsymbol{t}$, the desired result follows then immediately. □

Chapter 4

Discrepancy estimates for the acceptance-rejection sampler using stratified inputs

4.1 Introduction

In this chapter, we propose an acceptance-rejection sampler using stratified inputs as the driver sequence. We estimate the discrepancy of the N-point set in $(s-1)$-dimension generated by the proposed algorithm. First we show an upper bound on the star-discrepancy of order $N^{-1/2-1/(2s)}$. Further we prove an upper bound on the q-th moment of the L_q-discrepancy $(\mathbb{E}[N^q L_{q,N}^q])^{1/q}$ for $2 \leq q \leq \infty$, which is of order $N^{(1-1/s)(1-1/q)}$. The proposed approach is numerically tested and compared with the standard acceptance-rejection algorithm using pseudo-random inputs. From our numerical experiments we can see that, adapting stratified inputs in the acceptance-rejection sampler outperforms the original algorithm. The numerical results are roughly in agreement with the upper bounds in Theorems 4.2.6 and 4.2.7.

The chapter is organized as follows. In Section 4.1 we provide the needed notation and background, and introduce the proposed acceptance-rejection sampler using stratified inputs. Section 4.2 focuses on the theoretical results including an

upper bound on the star-discrepancy and the L_q-discrepancy. Numerical tests are presented in Section 4.3 together with a discussion of the results in comparison with the theoretical bounds. For comparison purpose only, we do the numerical tests also with pseudo-random inputs. The chapter ends with the proofs of our main results and a short discussion.

4.1.1 Stratified sampling

Stratified sampling is one of the variance reduction methods used in Monte Carlo sampling. This method first splits the domain into smaller subsets and then puts a certain number of points in each smaller domain, see for instance [31, Chapter 4]. The use of stratified sampling depends on two aspects: working domain splitting and generating samples in each strata. The efficiency of stratified inputs has been well studied. The convergence analysis can refer to for instance [65, Chapter 10].

Stratified inputs are good for generating a uniformly distributed point set. In order to generate low-discrepancy samples with respect to non-uniform distribution, we can use stratification through the acceptance-rejection.

4.1.2 Acceptance-rejection sampler with stratified inputs

We now present the acceptance-rejection algorithm using stratified inputs.

Algorithm 4.1.1. *Let the target density $\psi : [0,1]^{s-1} \to \mathbb{R}_+$, where $s \geq 2$, be given. Assume that we know a constant $L < \infty$ such that $\psi(\boldsymbol{z}) \leq L$ for all $\boldsymbol{z} \in [0,1]^{s-1}$. Let $A = \{\boldsymbol{z} \in [0,1]^s : \psi(z_1, \ldots, z_{s-1}) \geq L z_s\}$.*

i) Let $M \in \mathbb{N}$ and let $\{Q_0, \ldots, Q_{M-1}\}$ be a disjoint covering of $[0,1)^s$ with Q_i of the form $\prod_{j=1}^{s} \left[\frac{c_j}{M^{1/s}}, \frac{c_j+1}{M^{1/s}}\right)$ with $0 \leq c_j \leq \lceil M^{1/s} \rceil - 1$. Then $\lambda(Q_i) = 1/M$ for all $0 \leq i \leq M-1$. Generate a point set $P_M = \{\boldsymbol{x}_0, \boldsymbol{x}_1 \ldots, \boldsymbol{x}_{M-1}\}$ such that $\boldsymbol{x}_i \in Q_i$ is uniformly distributed in the sub-cube Q_i for each $i = 0, 1, \ldots, M-1$.

ii) *Use the acceptance-rejection method for the points in P_M with respect to the density ψ, i.e. we accept the point $\boldsymbol{x}_n$ if $\boldsymbol{x}_n \in A$, otherwise reject. Let $Y_N^{(s)} = A \cap P_M = \{\boldsymbol{z}_0, \boldsymbol{z}_1 \ldots, \boldsymbol{z}_{N-1}\}$ be the sample set we accept.*

iii) *Project the points we accepted $Y_N^{(s)}$ onto the first $(s-1)$ coordinates. Let $Y_N^{(s-1)} = \{\boldsymbol{y}_0, \boldsymbol{y}_1 \ldots, \boldsymbol{y}_{N-1}\}$ be the projections of the points $Y_N^{(s)}$.*

iv) *Return the point set $Y_N^{(s-1)}$.*

Note that $M^{1/s}$ is not necessarily an integer in Algorithm 4.1.1 and hence the sets Q_i do not necessarily partition the unit cube $[0,1)^s$. The restriction that $M^{1/s}$ is an integer forces one to choose $M = K^s$ for some $K \in \mathbb{N}$, which grows fast for large s. However, this restriction is not necessary and hence we do not assume here that $M^{1/s}$ is an integer.

As the main goal of our research, we are interested in the discrepancy properties of points produced by the acceptance-rejection method with stratified inputs as driver sequence. We prove bounds on the L_q-discrepancy and the star-discrepancy. In particular, in the numerical tests we calculate the L_2-discrepancy and star-discrepancy of the obtained samples.

By Definition 2.1.3, for a point set $P_N = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N-1}\}$ in $[0,1]^s$, the L_2-discrepancy is given by

$$L_2(P_N) = \left(\int_{[0,1]^s} \left| \frac{1}{N} \sum_{n=0}^{N-1} 1_{[\boldsymbol{0},\boldsymbol{t})}(\boldsymbol{x}_n) - \lambda([\boldsymbol{0},\boldsymbol{t})) \right|^2 \mathrm{d}\boldsymbol{t} \right)^{1/2}.$$

The reason we are particularly interested in the L_2-discrepancy is because there is a concise formula for the L_2-discrepancy due to Warnock [85].

Proposition 4.1.2. *For any point set $P_N = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N-1}\}$ in $[0,1]^s$, we have*

$$L_{2,N}^2(P_N) = \frac{1}{3^s} - \frac{2}{N} \sum_{n=0}^{N-1} \prod_{i=1}^{s} \frac{1 - x_{n,i}^2}{2} + \frac{1}{N^2} \sum_{m,n=0}^{N-1} \prod_{i=1}^{s} \min(1 - x_{m,i}, 1 - x_{n,i}),$$

where $x_{n,i}$ is the i-th component of the point $\boldsymbol{x}_n$.

Later we will present a closed formula for the L_2-discrepancy of samples associated with a density function.

This proposition can be derived from Equation (2.3.2), the formula representing the worst-case error for a reproducing kernel Hilbert space, by choosing the reproducing kernel $K(\boldsymbol{x},\boldsymbol{y}) = \prod_{j=1}^{s} \min\{1-x_j, 1-y_j\}$.

Now we extend the formula to the non-uniform case. Let $\psi : [0,1]^{s-1} \to \mathbb{R}_+$ be a density function, let $C = \int_{[0,1]^{s-1}} \psi(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} > 0$ and $s \geq 2$. The L_2-discrepancy of samples $Y_N^{(s-1)} \subset [0,1]^{s-1}$ with respect to ψ is given as follows,

$$L_2(Y_N^{(s-1)}, \psi) = \Big(\int_{[0,1]^{s-1}} \Big| \frac{1}{N} \sum_{n=0}^{N-1} 1_{[\mathbf{0},\boldsymbol{t})}(\boldsymbol{y}_n) - \frac{1}{C} \int_{[\mathbf{0},\boldsymbol{t})} \psi(\boldsymbol{z}) d\boldsymbol{z} \Big|^2 \mathrm{d}\boldsymbol{t} \Big)^{1/2},$$

where $\boldsymbol{t} = (t_1, \ldots, t_{s-1})$.

A representation of the L_2-discrepancy in terms of the non-uniform density ψ can be obtained as follows. Let

$$\Delta_{\psi,\boldsymbol{t}} = \Big| \frac{1}{N} \sum_{n=0}^{N-1} 1_{[\mathbf{0},\boldsymbol{t})}(\boldsymbol{y}_n) - \frac{1}{C} \int_{[\mathbf{0},\boldsymbol{t})} \psi(\boldsymbol{z}) d\boldsymbol{z} \Big|,$$

then

$$\begin{aligned} \Delta_{\psi,\boldsymbol{t}}^2 &= \Big| \frac{1}{N} \sum_{n=0}^{N-1} 1_{[\mathbf{0},\boldsymbol{t})}(\boldsymbol{y}_n) - \frac{1}{C} \int_{[\mathbf{0},\boldsymbol{t})} \psi(\boldsymbol{z}) d\boldsymbol{z} \Big|^2 \\ &= \frac{1}{N^2} \sum_{m,n=0}^{N-1} \prod_{j=1}^{s-1} 1_{[0,t_j)}(\max\{y_{m,j}, y_{n,j}\}) + \frac{(\int_{[\mathbf{0},\boldsymbol{t})} \psi(\boldsymbol{z}) d\boldsymbol{z})^2}{C^2} \\ &\quad - \frac{2}{NC} \sum_{i=0}^{N-1} \prod_{j=1}^{s-1} 1_{[0,t_j)}(y_{i,j}) \int_{[\mathbf{0},\boldsymbol{t})} \psi(\boldsymbol{z}) d\boldsymbol{z}. \end{aligned}$$

Therefore the squared L_2-discrepancy associated with density ψ is given by

$$\begin{aligned} & L_2(Y_N^{(s-1)}, \psi)^2 \\ = & \int_{[0,1]^{s-1}} \Delta_{\psi,\boldsymbol{t}}^2 \,\mathrm{d}\boldsymbol{t} \\ = & \frac{1}{N^2} \sum_{m,n=0}^{N-1} \prod_{j=1}^{s-1} (1 - \max\{y_{m,j}, y_{n,j}\}) + \frac{1}{C^2} \int_{[0,1]^{s-1}} \Big(\int_{[\mathbf{0},\boldsymbol{t})} \psi(\boldsymbol{z}) d\boldsymbol{z} \Big)^2 \mathrm{d}\boldsymbol{t} \\ & - \frac{2}{NC} \int_{[0,1]^{s-1}} \int_{[\mathbf{0},\boldsymbol{t})} \sum_{i=0}^{N-1} \prod_{j=1}^{s-1} 1_{[0,t_j)}(y_{i,j}) \psi(\boldsymbol{z}) d\boldsymbol{z}\, \mathrm{d}\boldsymbol{t}. \end{aligned} \tag{4.1.1}$$

In order to generate samples from the density function ψ, we employ the acceptance-rejection algorithm. The acceptance-rejection algorithm accepts all points

below the graph of the density function with a well-chosen but simple proposal density.

For our proof, we again assume that the set below the graph of the density function admits a so-called Minkowski content as we introduced in Section 3.2.4. For completeness we recall the concept here, see also Definition 3.2.11. For a set $A \subseteq \mathbb{R}^s$, let ∂A denote the boundary of A and let

$$\mathcal{M}(\partial A) = \lim_{\varepsilon \to 0} \frac{\lambda((\partial A)_\varepsilon)}{2\varepsilon},$$

where $(\partial A)_\varepsilon = \{\boldsymbol{x} \in \mathbb{R}^s | \|\boldsymbol{x} - \boldsymbol{y}\| \leq \varepsilon \text{ for } \boldsymbol{y} \in \partial A\}$ and $\|\cdot\|$ denotes the Euclidean norm. If $\mathcal{M}(\partial A)$ (abbreviated as $\mathcal{M}_A$) exists and is finite, then ∂A is said to admit an $(s-1)-$dimensional Minkowski content.

4.2 Discrepancy estimates

We present some results that we use to prove an upper bound for the star-discrepancy with respect to points generated by the acceptance-rejection sampler using stratified inputs.

The concept of δ-cover is a very useful technique used in approximating the star-discrepancy, see Section 3.4 for the definition and relevant discussion. The following result on the size of the δ-cover is obtained from [32, Theorem 1.15].

Lemma 4.2.1. *For any $s \in \mathbb{N}$ and $\delta > 0$ there exists a δ-cover of the set of anchored boxes $[\mathbf{0}, \boldsymbol{t}) \subseteq [0,1)^s$ which has cardinality at most $(2e)^s(\delta^{-1}+1)^s$.*

By a simple generalization, the following result holds for our setting.

Lemma 4.2.2. *Let $\psi : [0,1]^{s-1} \to \mathbb{R}_+$, where $s \geq 2$, be a function. Assume that there exists a constant $L < \infty$ such that $\psi(\boldsymbol{z}) \leq L$ for all $\boldsymbol{z} \in [0,1]^{s-1}$. Let $A = \{\boldsymbol{z} \in [0,1]^s : \psi(z_1, \ldots, z_{s-1}) \geq L z_s\}$ and $J_{\boldsymbol{t}}^* = ([\mathbf{0}, \boldsymbol{t}) \times [0,1]) \cap A$, for $\boldsymbol{t} \in [0,1]^{s-1}$. Let $(A, \mathcal{B}(A), \lambda)$ be a probability space where $\mathcal{B}(A)$ is the Borel σ-algebra of A. Define the set $\mathcal{A} \subset \mathcal{B}(A)$ of test sets by*

$$\mathcal{A} = \{J_{\boldsymbol{t}}^* : \boldsymbol{t} \in [0,1]^{s-1}\}.$$

Then for any $\delta > 0$ there exists a δ-cover Γ_δ of $\mathcal{A}$ with

$$|\Gamma_\delta| \leq (2e)^{s-1}(\delta^{-1}+1)^{s-1}.$$

Lemma 4.2.3. *Let the unnormalized density function $\psi : [0,1]^{s-1} \to \mathbb{R}_+$, with $s \geq 2$, be given. Assume that there exists a constant $L < \infty$ such that $\psi(\boldsymbol{z}) \leq L$ for all $\boldsymbol{z} \in [0,1]^{s-1}$.*

- *Let $M \in \mathbb{N}$ and let the subsets $Q_0, \ldots, Q_{M-1}$ be a disjoint covering of $[0,1)^s$ of the form $\prod_{i=1}^s \left[\frac{c_j}{M^{1/s}}, \frac{c_j+1}{M^{1/s}}\right)$ where $0 \leq c_j \leq \lceil M^{1/s} \rceil - 1$. Each set Q_i satisfies $\lambda(Q_i) = 1/M$.*
- *Let*

  $$A = \{\boldsymbol{z} \in [0,1]^s : \psi(z_1, \ldots, z_{s-1}) \geq L z_s\}.$$

  Assume that ∂A admits an $(s-1)-$dimensional Minkowski content $\mathcal{M}_A$.
- *Let $J_{\boldsymbol{t}}^* = ([\boldsymbol{0}, \boldsymbol{t}) \times [0,1]) \bigcap A$, where $\boldsymbol{t} = (t_1, \ldots, t_{s-1}) \in [0,1]^{s-1}$.*

Then there exists an $M_0 \in \mathbb{N}$ such that $\partial J_{\boldsymbol{t}}^*$ intersects at most with $3s^{1/2}\mathcal{M}_A M^{1-1/s}$ subcubes Q_i, for all $M \geq M_0$.

This result can be obtained utilizing a similar proof as in [36, Theorem 4.3]. For the sake of completeness, we give the proof here.

Proof. Since ∂A admits an $(s-1)-$dimensional Minkowski content, it follows that

$$\mathcal{M}_A = \lim_{\varepsilon \to 0} \frac{\lambda((\partial A)_\varepsilon)}{2\varepsilon} < \infty.$$

Thus by the definition of the limit, for any fixed $\vartheta > 2$, there exists $\varepsilon_0 > 0$ such that $\lambda((\partial A)_\varepsilon) \leq \vartheta \varepsilon \mathcal{M}_A$ whenever $0 < \varepsilon \leq \varepsilon_0$.

Based on the form of the subcube given by $\prod_{i=1}^s \left[\frac{c_j}{M^{1/s}}, \frac{c_j+1}{M^{1/s}}\right)$, the largest diagonal length is $\sqrt{s}M^{-1/s}$. We can assume that $M > (\sqrt{s}/\varepsilon_0)^s$, then $\sqrt{s}M^{-1/s} =: \varepsilon < \varepsilon_0$ and $\bigcup_{i \in J} Q_i \subseteq (\partial A)_\varepsilon$, where J is the index set for the sets Q_i which satisfy $Q_i \cap \partial A \neq \emptyset$. Therefore

$$|J| \leq \frac{\lambda((\partial A)_\varepsilon)}{\lambda(Q_i)} \leq \frac{\vartheta \varepsilon \mathcal{M}_A}{M^{-1}} = \sqrt{s}\vartheta \mathcal{M}_A M^{1-1/s}.$$

Without loss of generality, we can set $\vartheta = 3$. Note that the number of boxes Q_i which intersect $\partial J_{\boldsymbol{t}}^*$ is bounded by the number of boxes Q_i which intersect ∂A, which completes the proof. □

Remark. *Ambrosio et al. [4] found that for a closed set $A \subset \mathbb{R}^s$, if A has a Lipschitz boundary, then ∂A admits an $(s-1)$-dimensional Minkowski content. In particular, a convex set $A \subset [0,1]^s$ has an $(s-1)$-dimensional Minkowski content. Note that the surface area of a convex set in $[0,1]^s$ is bounded by the surface area of the unit cube $[0,1]^s$, which is $2s$ and it was also shown by Niederreiter and Wills [61] that $2s$ is best possible. It follows that the Minkowski content $\mathcal{M}_A \leq 2s$ when A is a convex set in $[0,1]^s$.*

Lemma 4.2.4. *Suppose that all the assumptions of Lemma 4.2.3 are satisfied. Let N be the number of points accepted by Algorithm 4.1.1. Then we have*

$$M(\lambda(A) - 3s^{1/2}\mathcal{M}_A M^{-1/s}) \leq N \leq M(\lambda(A) + 3s^{1/2}\mathcal{M}_A M^{-1/s}).$$

Proof. The number of points we accept in Algorithm 4.1.1 is a random number since the driver sequence given by stratified inputs is random. Let $\mathbb{E}(N)$ be the expectation of N. The number of Q_i which have non-empty intersection with ∂A is bounded by $l = 3s^{1/2}\mathcal{M}_A M^{1-1/s}$ from Lemma 4.2.3. Thus

$$\mathbb{E}[N] - l \leq N \leq \mathbb{E}[N] + l. \tag{4.2.1}$$

Further we have

$$\mathbb{E}[N] = \sum_{i=0}^{M-1} \frac{\lambda(Q_i \cap A)}{\lambda(Q_i)} = M\lambda(A). \tag{4.2.2}$$

Combining (4.2.1) and (4.2.2) and substituting $l = 3s^{1/2}\mathcal{M}_A M^{1-1/s}$, one obtains the desired result. □

Before we state the upper bound on the star-discrepancy, our proof method requires the well-known Bernstein-Chernoff inequality.

Lemma 4.2.5. *([8, Lemma 2]). Let $\eta_0, \ldots, \eta_{l-1}$ be independent random variables with $\mathbb{E}(\eta_i) = 0$ and $|\eta_i| \leq 1$ for all $0 \leq i \leq l-1$. Denote by σ_i^2 the variance of η_i,*

i.e. $\sigma_i^2 = \mathbb{E}(\eta_i^2)$. *Set* $\beta = (\sum_{i=0}^{l-1} \sigma_i^2)^{1/2}$. *Then for any* $\gamma > 0$ *we have*

$$\mathbb{P}\left(\Big| \sum_{i=0}^{l-1} \eta_i \Big| \geq \gamma \right) \leq \begin{cases} 2e^{-\gamma/4}, & \text{if } \gamma \geq \beta^2, \\ 2e^{-\gamma^2/4\beta^2}, & \text{if } \gamma \leq \beta^2. \end{cases}$$

4.2.1 Existence result of samples with small star-discrepancy

The star-discrepancy of samples $Y_N^{(s-1)}$ obtained by Algorithm 4.1.1 with respect to the target density ψ is given as follows,

$$D^*_{N,\psi}(Y_N^{(s-1)}) = \sup_{\boldsymbol{t} \in [0,1]^{s-1}} \Big| \frac{1}{N} \sum_{n=0}^{N-1} 1_{[\mathbf{0},\boldsymbol{t})}(\boldsymbol{y}_n) - \frac{1}{C} \int_{[\mathbf{0},\boldsymbol{t})} \psi(\boldsymbol{z}) d\boldsymbol{z} \Big|,$$

where $C = \int_{[0,1]^{s-1}} \psi(\boldsymbol{z})\, \mathrm{d}\boldsymbol{z} > 0$ and $s \geq 2$.

We can prove the following result for samples generated by the acceptance-rejection sampler with stratified inputs.

Theorem 4.2.6. *Let an unnormalized density function* $\psi : [0,1]^{s-1} \to \mathbb{R}_+$, *with* $s \geq 2$, *be given. Assume that there exists a constant* $L < \infty$ *such that* $\psi(\boldsymbol{z}) \leq L$ *for all* $\boldsymbol{z} \in [0,1]^{s-1}$. *Let* $C = \int_{[0,1]^{s-1}} \psi(\boldsymbol{z})\, \mathrm{d}\boldsymbol{z} > 0$ *and let the graph under* ψ *be defined as*

$$A = \{\boldsymbol{z} \in [0,1]^s : \psi(z_1, \ldots, z_{s-1}) \geq L z_s\}.$$

Assume that ∂A *admits an* $(s-1)-$*dimensional Minkowski content* $\mathcal{M}_A$. *Then for all large enough* N, *with positive probability, Algorithm 4.1.1 yields a point set* $Y_N^{(s-1)} \subseteq [0,1]^{s-1}$ *such that*

$$D^*_{N,\psi}(Y_N^{(s-1)}) \leq \frac{s^{\frac{3}{4}} \sqrt{6\mathcal{M}_A}}{2^{\frac{1}{2s}-\frac{1}{2}} (\lambda(A))^{\frac{1}{2}-\frac{1}{2s}}} \frac{\sqrt{\log N}}{N^{\frac{1}{2}+\frac{1}{2s}}} + \frac{2\lambda(A)}{N}, \tag{4.2.3}$$

where $\lambda(A) = C/L$.

Roughly speaking, the stratified inputs combined with the acceptance-rejection technique yields that the star-discrepancy of the corresponding samples is bounded by $N^{-1/2-1/2s}$, which is slightly better than the rate of plain Monte Carlo. The proof of this upper bound on the star-discrepancy is presented in Section 4.4.1.

4.2.2 Upper bound on the L_q-discrepancy

In this section we provide an upper bound on the expected value of the L_q-discrepancy for $2 \le q \le \infty$. We establish an upper bound for $\big(\mathbb{E}[N^q L_{q,N}^q(Y_N^{(s-1)})]\big)^{1/q}$ which is given by

$$\Big(\mathbb{E}\Big[N^q L_{q,N}^q(Y_N^{(s-1)})\Big]\Big)^{1/q} = \left(\mathbb{E}\Big[\int_{[0,1)^{s-1}} \Big|\sum_{n=0}^{N-1} 1_{[\mathbf{0},\boldsymbol{t})}(\boldsymbol{y}_n) - \frac{N}{C}\int_{[\mathbf{0},\boldsymbol{t})} \psi(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z}\Big|^q \,\mathrm{d}\boldsymbol{t}\Big]\right)^{1/q},$$

where $Y_N^{(s-1)}$ is the sample set associated with the density function ψ.

Theorem 4.2.7. *Let the unnormalized density function $\psi : [0,1]^{s-1} \to \mathbb{R}_+$ satisfy all the assumptions stated in Theorem 4.2.6. Let $Y_N^{(s-1)}$ be the samples generated by the acceptance-rejection sampler using stratified inputs in Algorithm 4.1.1. Then we have for $2 \le q \le \infty$,*

$$\big(\mathbb{E}[N^q L_{q,N}^q(Y_N^{(s-1)})]\big)^{1/q} \le \frac{2^{(1-1/s)(1-1/q)}(3s^{1/2}\mathcal{M}_A)^{1-1/q}}{4\sqrt{2}C(\lambda(A))^{(1-1/s)(1-1/q)}} N^{(1-1/s)(1-1/q)}, \qquad (4.2.4)$$

where $\mathcal{M}_A$ is the $(s-1)$-dimensional Minkowski content and the expectation is taken with respect to the stratified inputs.

In this theorem we can see that $(\mathbb{E}[N^q L_{q,N}^q])^{1/q}$ achieves an order of convergence of $N^{(1-1/s)(1-1/q)}$ for $2 \le q \le \infty$. We defer the proof to Section 4.4.2. Basically we prove upper bounds for L_2-discrepancy and L_∞-discrepancy (i.e. star-discrepancy) respectively, then use interpolation for the case $2 < q < \infty$. It would also be interesting to find out whether (4.2.4) still holds for $1 < q < 2$. See Heinrich [37] for a possible proof technique. We leave it as an open problem.

4.3 Numerical results

We consider the discrepancy of samples generated by Algorithm 4.1.1 with respect to the given density ψ defined by

$$\psi(x_1,x_2,x_3,x_4) = \frac{1}{4}(e^{-x_1}+e^{-x_2}+e^{-x_3}+e^{-x_4}), \quad (x_1,x_2,x_3,x_4) \in [0,1]^4.$$

To compute the star-discrepancy, we utilize the same technique as presented in Section 3.4, a so-called δ-cover, to estimate the supremum in the definition of the star-discrepancy. We also calculate the L_2-discrepancy of samples for this example. The L_2-discrepancy with respect to a density function is denoted by,

$$L_2(Y_N^{(s-1)},\psi) = \Big(\int_{[0,1]^{s-1}} \Big|\frac{1}{N}\sum_{n=0}^{N-1} 1_{[\mathbf{0},\boldsymbol{t})}(\boldsymbol{y}_n) - \frac{1}{C}\int_{[\mathbf{0},\boldsymbol{t})} \psi(\boldsymbol{z})d\boldsymbol{z}\Big|^2 \,\mathrm{d}\boldsymbol{t}\Big)^{1/2}, \qquad (4.3.1)$$

where $C = \int_{[0,1]^{s-1}} \psi(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} > 0$ and $\boldsymbol{t} = (t_1,\dots,t_{s-1})$. One can write down a precise formula for the squared L_2-discrepancy for a given ψ in this example according to Equation 4.1.1, which is

$$\begin{aligned} L_2(Y_N^{(s-1)},\psi)^2 \;=\; & \frac{1}{N^2}\sum_{m,n=0}^{N-1}\prod_{j=1}^{s-1}(1-\max\{y_{m,j},y_{n,j}\}) + \frac{1}{4C^2}\Big(\frac{71}{54e^2} - \frac{16}{27e} + \frac{7}{108}\Big) \\ & -\frac{1}{16NC}\sum_{i=0}^{N-1}\sum_{j=1}^{4}(1+e^{-1}-y_{i,j}-e^{-y_{i,j}})\frac{\prod_{k=1}^{4}(1-y_{i,k}^2)}{1-y_{i,j}^2}, \end{aligned}$$

where $C = 1 - 1/e$.

Theorem 4.2.6 shows that Algorithm 4.1.1 can yield a point set satisfying the discrepancy bound (4.2.3). To test this result numerically and to compare it to the acceptance-rejection algorithm using random inputs, we perform the following numerical test. We generate 100 independent stratified inputs and 100 independent pseudo-random inputs for the acceptance-rejection algorithm. From the sample sets obtained from the acceptance-rejection algorithm we choose those samples which yield the fastest rate of convergence for stratified inputs and also for pseudo-random inputs. Note that the numerical results in the follows figures are presented in a log-log scale.

Theorem 4.2.6 suggests a convergence rate of order $N^{-1/2-1/(2s)} = N^{-0.6}$ for stratified inputs. The numerical results in this test shows an empirical convergence of $N^{-0.62}$, see Figure 4.1. In comparison, the same test carried out with the stratified inputs replaced by pseudo-random inputs shows a convergence rate of order $N^{-0.55}$. As expected, stratified inputs outperform random inputs.

We also perform numerical experiments to test Theorem 4.2.7. For $q = \infty$, the left side in (4.2.4) is the infinite moment, i.e. the essential supremum, of the random

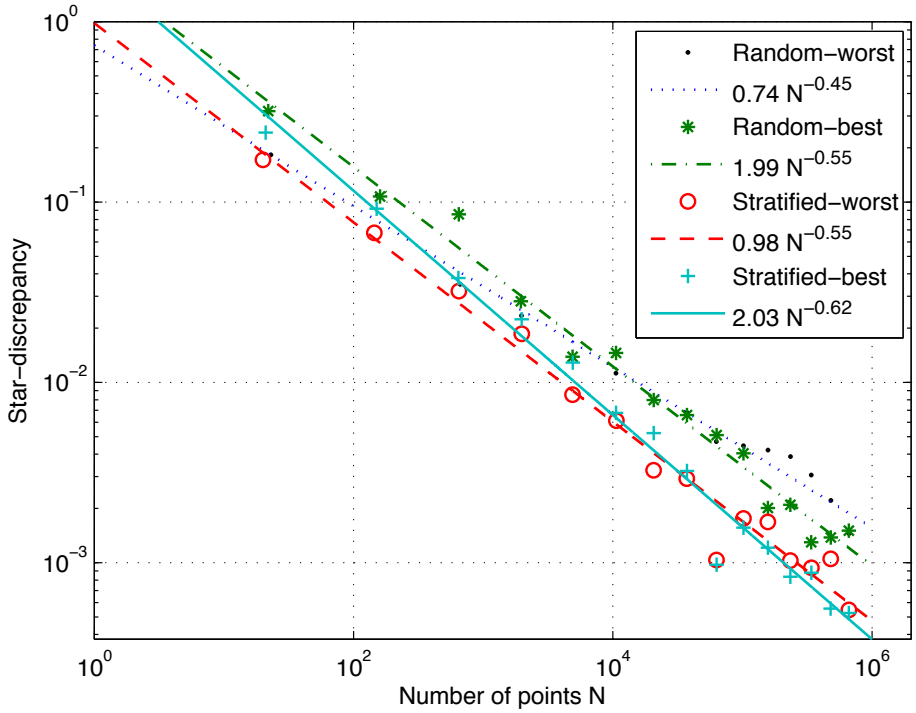


Figure 4.1: Convergence order of the star-discrepancy with stratified inputs.

variable $NL_{q,N}(Y_N^{s-1})$. Theorem 4.2.7 suggests a convergence rate of order $N^{-1/s} = N^{-0.2}$. To compare this result with the numerical performance in our example, we use again 100 independent runs, but now choose the one with the worst convergence rate for each case. With stratified inputs, we get a convergence rate of order $N^{-0.55}$ in this case (see Figure 4.1), which may suggest that Theorem 4.2.7 is too pessimistic. Note that Theorem 4.2.7 only requires very weak smoothness assumptions on the target density, whereas the density in our example is very smooth. This may explain the difference between the theoretical and numerical results.

We also test Theorem 4.2.7 for the case $q = 2$. In this case, the left side of (4.2.4) is an L_2 average of $NL_{2,N}(Y_N^{s-1})$. Theorem 4.2.7 with $q = 2$ suggests a convergence rate of $L_{2,N}(Y_N^{s-1})$ of order $N^{-1/2-1/(2s)} = N^{-0.6}$. The numerical experiment in Figure 4.2 yields a convergence rate of order $N^{-0.59}$, roughly in agreement with Theorem 4.2.7 for $q = 2$. For random inputs we get a convergence rate of order

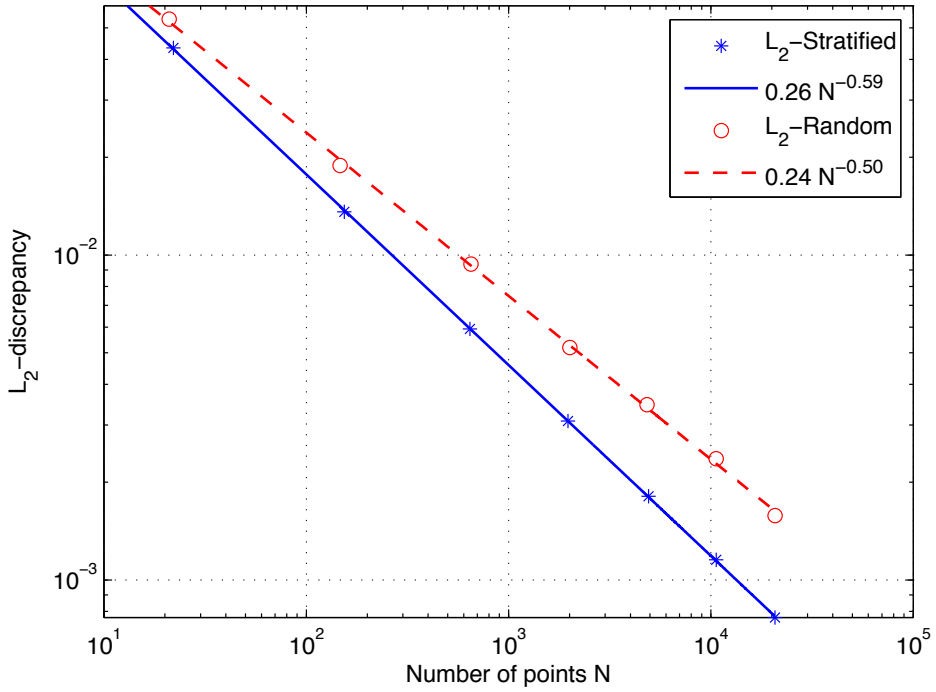


Figure 4.2: Convergence order of the L_2-discrepancy with stratified inputs.

$N^{-0.50}$, as one would expect.

4.4 Proofs

4.4.1 Proof of Theorem 4.2.6

Proof. Let $J_{\boldsymbol{t}}^* = ([\mathbf{0}, \boldsymbol{t}) \times [0,1]) \bigcap A$, where $\boldsymbol{t} = (t_1, \ldots, t_{s-1})$. Using the notation from Algorithm 4.1.1, let $\boldsymbol{y}_n$ be the first $s-1$ coordinates of $\boldsymbol{z}_n \in A$, for $n = 0, \ldots, N-1$. We have

$$\sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) = \sum_{n=0}^{N-1} 1_{[\mathbf{0},\boldsymbol{t})}(\boldsymbol{y}_n).$$

Therefore

$$\left|\frac{1}{N}\sum_{n=0}^{N-1} 1_{[\mathbf{0},\boldsymbol{t})}(\boldsymbol{y}_n) - \frac{1}{C}\int_{[\mathbf{0},\boldsymbol{t})} \psi(\boldsymbol{z}) d\boldsymbol{z}\right| = \left|\frac{1}{N}\sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) - \frac{1}{\lambda(A)}\lambda(J_{\boldsymbol{t}}^*)\right|. \quad (4.4.1)$$

It is noted that

$$\begin{aligned}\Big|\sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) - \frac{N}{\lambda(A)}\lambda(J_{\boldsymbol{t}}^*)\Big| &\leq \Big|\sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) - M\lambda(J_{\boldsymbol{t}}^*)\Big| + \Big|\lambda(J_{\boldsymbol{t}}^*)\big(M - \frac{N}{\lambda(A)}\big)\Big| \\ &\leq \Big|\sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) - M\lambda(J_{\boldsymbol{t}}^*)\Big| + \Big|M\lambda(A) - N\Big| \\ &\leq \Big|\sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) - M\lambda(J_{\boldsymbol{t}}^*)\Big| + \Big|M\lambda(A) - \sum_{n=0}^{M-1} 1_A(\boldsymbol{x}_n)\Big| \\ &\leq 2\sup_{\boldsymbol{t}\in[0,1]^s}\Big|\sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) - M\lambda(J_{\boldsymbol{t}}^*)\Big|. \qquad (4.4.2)\end{aligned}$$

Let us associate with each Q_i, random points $\boldsymbol{x}_i \in Q_i$ with probability distribution

$$\mathbb{P}(\boldsymbol{x}_i \in V) = \frac{\lambda(V)}{\lambda(Q_i)} = M\lambda(V),$$

for all measurable sets $V \subseteq Q_i$.

It follows from Lemma 4.2.3 that $\partial J_{\boldsymbol{t}}^*$ intersects at most $l := 3s^{1/2}\mathcal{M}_A M^{1-1/s}$ sets Q_i. Therefore, $J_{\boldsymbol{t}}^*$ is representable as the disjoint union of sets Q_i entirely contained in $J_{\boldsymbol{t}}^*$ and the union of at most l sets Q_i for which $Q_i \cap J_{\boldsymbol{t}}^* \neq \emptyset$ and $Q_i \cap ([0,1]^s \setminus J_{\boldsymbol{t}}^*) \neq \emptyset$, i.e.

$$J_{\boldsymbol{t}}^* = \bigcup_{i\in I} Q_i \cup \bigcup_{i\in J}(Q_i \cap J_{\boldsymbol{t}}^*),$$

where the index-set J has cardinality at most $\lceil 3s^{1/2}\mathcal{M}_A M^{1-1/s}\rceil$. Since for every Q_i, $\lambda(Q_i) = 1/M$ and $\boldsymbol{x}_i \in Q_i$ for $i = 0, 1, \ldots, M-1$, the discrepancy of $\bigcup_{i\in I} Q_i$ is zero. Therefore, it remains to investigate the discrepancy of $\bigcup_{i\in J}(Q_i \cap J_{\boldsymbol{t}}^*)$.

Since $\lambda(A) = C/L$ and $N \geq M(C/L - 3s^{1/2}\mathcal{M}_A M^{-1/s})$ by Lemma 4.2.4, we have $M \leq 2LN/C$ for all $M > (6Ls^{1/2}\mathcal{M}_A/C)^s$. Consequently,

$$l = 3s^{1/2}\mathcal{M}_A M^{1-1/s} \leq 3s^{1/2}(2L)^{1-1/s}C^{1/s-1}\mathcal{M}_A N^{1-\frac{1}{s}} = \Omega N^{1-1/s},$$

where $\Omega = 3s^{1/2}(2L)^{1-1/s}C^{1/s-1}\mathcal{M}_A$.

Let us define the random variable χ_i for $0 \leq i \leq l-1$ as follows

$$\chi_i = \begin{cases} 1, & \text{if } \boldsymbol{z}_i \in Q_i \cap J_{\boldsymbol{t}}^*, \\ 0, & \text{if } \boldsymbol{z}_i \notin Q_i \cap J_{\boldsymbol{t}}^*. \end{cases}$$

By definition,

$$\Big|\sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) - M\lambda(J_{\boldsymbol{t}}^*)\Big| = \Big|\sum_{i=0}^{l-1}\chi_i - M\sum_{i=0}^{l-1}\lambda(Q_i\cap J_{\boldsymbol{t}}^*)\Big|. \tag{4.4.3}$$

Because of $\mathbb{P}(\chi_i=1)=\lambda(Q_i\cap J_{\boldsymbol{t}}^*)/\lambda(Q_i)=M\lambda(Q_i\cap J_{\boldsymbol{t}}^*)$, we have

$$\mathbb{E}\chi_i = M\lambda(Q_i\cap J_{\boldsymbol{t}}^*), \tag{4.4.4}$$

where $\mathbb{E}[\cdot]$ denotes the expected value. By (4.4.3) and (4.4.4),

$$\Delta_N(J_{\boldsymbol{t}}^*;\boldsymbol{z}_1,\dots,\boldsymbol{z}_N) = \Big|\sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) - M\lambda(J_{\boldsymbol{t}}^*)\Big| = \Big|\sum_{i=0}^{l-1}(\chi_i-\mathbb{E}\chi_i)\Big|. \tag{4.4.5}$$

Since the random variables χ_i for $0\le i\le l-1$ are independent of each other, in order to estimate the sum $\sum_{i=0}^{l-1}(\chi_i-\mathbb{E}\chi_i)$ we are able to apply the classical Bernstein-Chernoff inequality of large deviation type. Let $\sigma_i^2=\mathbb{E}[\chi_i-\mathbb{E}\chi_i]^2$ and set $\beta=(\sum_{i=1}^{l}\sigma_i^2)^{1/2}$. Let

$$\gamma = \theta l^{1/2}(\log N)^{1/2},$$

where θ is a constant depending only on the dimension s which will be fixed later. Without loss of generality, assume that $N\ge 3$.

Case 1: If $\gamma\le\beta^2$, since $\beta^2\le l\le \Omega N^{1-\frac{1}{s}}$, by Lemma 4.2.5 we obtain

$$\begin{aligned}&\mathbb{P}\left(\Delta_N(J_{\boldsymbol{t}}^*;\boldsymbol{z}_1,\dots,\boldsymbol{z}_N)\ge\theta l^{1/2}(\log N)^{1/2}\right)\\ &=\mathbb{P}\Big(\Big|\sum_{i=1}^{l}(\chi_i-\mathbb{E}\chi_i)\Big|\ge\gamma\Big)\le 2e^{-\gamma^2/(4\beta^2)}\le 2N^{-\theta^2/4}.\end{aligned} \tag{4.4.6}$$

Though the class of axis-parallel boxes is uncountable, it suffices to consider a small subclass. Based on the argument in Lemma 4.2.2, there is an $1/M$-cover of cardinality $(2e)^{s-1}(M+1)^{s-1}\le(2e)^{s-1}(2LN/C+1)^{s-1}$ for $M>M_0$ such that there exist $R_1,R_2\in\Gamma_{1/M}$ having the properties $R_1\subseteq J_{\boldsymbol{t}}^*\subseteq R_2$ and $\lambda(R_2\setminus R_1)\le 1/M$. From this it follows that

$$\Delta_N(J_{\boldsymbol{t}}^*;\boldsymbol{z}_1,\dots,\boldsymbol{z}_N)\le\max_{i=1,2}\Delta(R_i;\boldsymbol{z}_1,\dots,\boldsymbol{z}_N)+1,$$

see, for instance, [26, Lemma 3.1] and [38, Section 2.1]. This means that we can restrict ourselves to the elements in $\Gamma_{1/M}$.

In view of (4.4.6)

$$\mathbb{P}\big(\Delta(R_i;\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)\geq\gamma\big)\leq|\Gamma_{1/M}|2N^{-\frac{\theta^2}{4}}\leq 2N^{-\frac{\theta^2}{4}}(2e)^{s-1}\big(\frac{2LN}{C}+1\big)^{s-1}<1,$$

for $\theta=2\sqrt{2s}$ and $N\geq\frac{8e}{C}+2$.

Case 2: On the other hand, if $\gamma\geq\beta^2$, then by Lemma 4.2.5 we obtain

$$\begin{aligned}&\mathbb{P}\Big(\Delta(J_{\boldsymbol{t}}^*;\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)\geq\theta l^{1/2}(\log N)^{1/2}\Big)\\&=\mathbb{P}\Big(\big|\sum_{i=1}^{l}(\chi_i-\mathbb{E}\chi_i)\big|\geq\gamma\Big)\leq 2e^{-\frac{\theta l^{1/2}(\log N)^{1/2}}{4}}.\end{aligned}\tag{4.4.7}$$

Similarly, using the $1/M$-cover above, for $\theta=2\sqrt{2s}$ and sufficiently large N we have

$$\begin{aligned}\mathbb{P}\big(\Delta(R_i;\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)\geq\gamma\big)&\leq|\Gamma_{1/M}|2e^{-\frac{\theta l^{1/2}(\log N)^{1/2}}{4}}\\&\leq 2e^{-\frac{\theta l^{1/2}(\log N)^{1/2}}{4}}(2e)^{s-1}\big(\frac{2LN}{C}+1\big)^{s-1}<1,\end{aligned}$$

where the last equation is satisfied for all large enough N.

By (4.4.1) and (4.4.2), we obtain that, with positive probability, Algorithm 4.1.1 yields a point set $Y_N^{(s-1)}$ such that

$$D_{N,\psi}^*(Y_N^{(s-1)})\leq\sqrt{2s}\Omega^{1/2}N^{-\frac{1}{2}-\frac{1}{2s}}(\log N)^{1/2}+1/M.$$

By Lemma 4.2.1, we have $1/M\leq 2C/(LN)$ for sufficiently large N. Thus the proof of Theorem 4.2.6 is complete. □

4.4.2 Proof of Theorem 4.2.7

Proof. Let $J_{\boldsymbol{t}}^*=([\mathbf{0},\boldsymbol{t})\times[0,1])\bigcap A$, where $\boldsymbol{t}=(t_1,\ldots,t_{s-1})\in[0,1]^{s-1}$. Let

$$\xi_i(\boldsymbol{t})=1_{Q_i\cap J_{\boldsymbol{t}}^*}(\boldsymbol{x}_i)-\lambda(Q_i\cap J_{\boldsymbol{t}}^*)/\lambda(Q_i),$$

where Q_i for $0\leq i\leq M-1$ is a disjoint covering of $[0,1)^s$ with $\lambda(Q_i)=1/M$. Then $\mathbb{E}[\xi_i(\boldsymbol{t})]=0$ since we have $\mathbb{E}[1_{Q_i\cap J_{\boldsymbol{t}}^*}(\boldsymbol{x}_i)]=M\lambda(Q_i\cap J_{\boldsymbol{t}}^*)$. Hence for any $\boldsymbol{t}\in[0,1]^{s-1}$,

$$\begin{aligned}\mathbb{E}[\xi_i^2(\boldsymbol{t})]&=\mathbb{E}[(1_{Q_i\cap J_{\boldsymbol{t}}^*}(\boldsymbol{x}_i)-M\lambda(Q_i\cap J_{\boldsymbol{t}}^*))^2]\\&=\mathbb{E}[1_{Q_i\cap J_{\boldsymbol{t}}^*}(\boldsymbol{x}_i)]-2M\lambda(Q_i\cap J_{\boldsymbol{t}}^*)\mathbb{E}[1_{Q_i\cap J_{\boldsymbol{t}}^*}(\boldsymbol{x}_i)]+M^2\lambda^2(Q_i\cap J_{\boldsymbol{t}}^*)\\&=M\lambda(Q_i\cap J_{\boldsymbol{t}}^*)(1-M\lambda(Q_i\cap J_{\boldsymbol{t}}^*))\leq 1/4.\end{aligned}$$

If $Q_i \subseteq J_{\boldsymbol{t}}^*$ or if $Q_i \cap J_{\boldsymbol{t}}^* = \emptyset$, we have $\xi_i(\boldsymbol{t}) = 0$. We order the sets Q_i such that $Q_0, Q_1, \ldots, Q_{i_0}$ satisfy $Q_i \cap J_{\boldsymbol{t}}^* \neq \emptyset$ and $Q_i \nsubseteq J_{\boldsymbol{t}}^*$ (i.e. Q_i intersects the boundary of $J_{\boldsymbol{t}}^*$) and the remaining sets Q_i either satisfy $Q_i \cap J_{\boldsymbol{t}}^* = \emptyset$ or $Q_i \subseteq J_{\boldsymbol{t}}^*$. If ∂A admits an $(s-1)$-dimensional Minkowski content, it follows from Lemma 4.2.3 that,

$$\sum_{i=0}^{M-1} \xi_i^2(\boldsymbol{t}) = \sum_{i=0}^{l-1} \xi_i^2(\boldsymbol{t}) \leq l/4 \text{ for all } \boldsymbol{t} \in [0,1]^{s-1}.$$

Again, $\mathbb{E}[N] = M\lambda(A)$ from Equation (4.2.2). Now for $q = 2$,

$$\begin{aligned}
&\Big(\mathbb{E}\Big[N^2 L_{2,N}^2(Y_N^{(s-1)})\Big]\Big)^{1/2} \\
&= \Big(\mathbb{E}\Big[\int_{[0,1)^{s-1}} \Big|\sum_{n=0}^{N-1} 1_{[\boldsymbol{0},\boldsymbol{t})}(\boldsymbol{y}_n) - \frac{N}{C}\int_{[\boldsymbol{0},\boldsymbol{t})} \psi(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z}\Big|^2 \mathrm{d}\boldsymbol{t}\Big]\Big)^{1/2} \\
&= \Big(\mathbb{E}\Big[\int_{[0,1)^{s-1}} \Big|\sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) - \frac{N\lambda(J_{\boldsymbol{t}}^*)}{\lambda(A)}\Big|^2 \mathrm{d}\boldsymbol{t}\Big]\Big)^{1/2} \\
&\leq \Big(\mathbb{E}\Big[\int_{[0,1)^{s-1}} \Big(\Big|\sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) - M\lambda(J_{\boldsymbol{t}}^*)\Big| + \Big|\frac{\mathbb{E}(N)\lambda(J_{\boldsymbol{t}}^*)}{\lambda(A)} - \frac{N\lambda(J_{\boldsymbol{t}}^*)}{\lambda(A)}\Big|\Big)^2 \mathrm{d}\boldsymbol{t}\Big]\Big)^{1/2} \\
&\leq \sqrt{2}\Big(\mathbb{E}\Big[\int_{[0,1)^{s-1}} \Big|\sum_{n=0}^{M-1} 1_{J_{\boldsymbol{t}}^*}(\boldsymbol{x}_n) - M\lambda(J_{\boldsymbol{t}}^*)\Big|^2 + \Big|\frac{\lambda(J_{\boldsymbol{t}}^*)}{\lambda(A)}(\mathbb{E}(N) - N)\Big|^2 \mathrm{d}\boldsymbol{t}\Big]\Big)^{1/2},
\end{aligned}$$

where we used $(a+b)^2 \leq 2(a^2+b^2)$.

Then we have

$$\begin{aligned}
\Big(\mathbb{E}\Big[N^2 L_{2,N}^2(Y_N^{(s-1)})\Big]\Big)^{1/2} &\leq \sqrt{2}\Big(\mathbb{E}\Big[\int_{[0,1]^{s-1}} \Big|\sum_{i=0}^{M-1} \xi_i(\boldsymbol{t})\Big|^2 \mathrm{d}\boldsymbol{t} + \frac{1}{(\lambda(A))^2}\big|\mathbb{E}(N) - N\big|^2\Big]\Big)^{1/2} \\
&= \sqrt{2}\Big(\int_{[0,1]^{s-1}} \mathbb{E}\Big[\sum_{i=0}^{M-1} \xi_i^2(t)\Big]\,\mathrm{d}\boldsymbol{t} + \frac{L^2}{C^2}\sum_{i=0}^{M-1} \xi_i^2(\boldsymbol{1})\Big)^{1/2} \\
&= \sqrt{2}\Big(\int_{[0,1]^{s-1}} \sum_{i=0}^{l-1} \mathbb{E}[\xi_i^2(t)]\,\mathrm{d}\boldsymbol{t} + \frac{L^2}{C^2}\sum_{i=0}^{l-1} \xi_i^2(\boldsymbol{1})\Big)^{1/2} \\
&\leq \sqrt{2}\Big(\frac{1}{4} + \frac{L^2}{C^2}\frac{l}{4}\Big)^{1/2} = \frac{(L^2+C^2)^{1/2}}{\sqrt{2}C} l^{1/2}.
\end{aligned}$$

Since $|\xi_i(t)| \leq 1$, for $q = \infty$, we have

$$\begin{aligned}
\sup_{P_M \subset [0,1]^s} |ND_N^*(Y_N^{(s-1)})| &= \sup_{P_M \subset [0,1]^s} \sup_{\boldsymbol{t} \in [0,1]^{s-1}} \Big|\sum_{i=0}^{M-1} \xi_i(\boldsymbol{t})\Big| = \sup_{P_M \subset [0,1]^s} \sup_{\boldsymbol{t} \in [0,1]^{s-1}} \Big|\sum_{i=0}^{l-1} \xi_i(\boldsymbol{t})\Big| \\
&\leq \sup_{P_M \in [0,1]^s} \sup_{\boldsymbol{t} \in [0,1]^{s-1}} \sum_{i=0}^{l-1} \big|\xi_i(\boldsymbol{t})\big| \leq l/4.
\end{aligned}$$

Therefore, for $2 \leq q \leq \infty$,

$$\left(\mathbb{E}[N^q L_{q,N}^q(Y_N^{(s-1)})]\right)^{1/q} \leq \frac{(L^2+C^2)^{1/2}}{4\sqrt{2}C} l^{1-1/q},$$

which is a consequence of the log-convexity of L_p-norms, i.e $\|f\|_{p_\theta} \leq \|f\|_{p_0}^{1-\theta}\|f\|_{p_1}^{\theta}$, where $1/p_\theta = (1-\theta)/p_0 + \theta/p_1$. In our case, $p_0 = 2$ and $p_1 = \infty$.

Additionally, following from Lemma 4.2.4, we have $M \leq 2LN/C$ whenever $M > (6Ls^{1/2}\mathcal{M}_A/C)^s$. Hence we obtain the desired result by substituting $l = 3s^{1/2}\mathcal{M}_A M^{1-1/s}$ and replacing M in terms of N. □

4.5 Remarks

Note that in some sense (t, m, s)-nets in base b are advanced stratified inputs where every type of elementary interval provides one way to decompose the domain $[0,1]^s$, and there are b^t points in each strata (see Figures 3.1 to 3.3 for illustrations of the corresponding decompositions of the unit square).

In Section 3.2.4, we proved a convergence rate of order $N^{-\alpha}$ for $1/s \leq \alpha < 1$ for samples generated by an acceptance-rejection sampler using (t, m, s)-nets as a driver sequence, where α depends on the target density ψ. One would expect an improvement of the convergence rate for stratified sampling. In order to obtain similar results for stratified inputs rather than (t, m, s)-nets, one would have to use the elementary intervals $U_1, \ldots, U_v$ of order k which yield a covering of $\partial J_{\boldsymbol{t}}^* \setminus \partial[0,1]^s$ for all $\boldsymbol{t} \in [0,1]^{s-1}$. From this covering one would then have to construct a covering of $\partial A \setminus \partial[0,1]^s$ and use this covering to obtain stratified inputs. In general, this strategy does not work with stratified sampling, unless one knows the elementary intervals explicitly. We did not pursue this approach further.

Chapter 5

Discrepancy bounds for deterministic acceptance-rejection samplers beyond $N^{-1/2}$

5.1 Background

In this chapter we consider an acceptance-rejection sampler based on deterministic driver sequences. We focus on the construction of good driver sequences which yield a small discrepancy of the sample set generated by the acceptance-rejection sampler.

We prove that the discrepancy of an N element sample set generated in this way is bounded by $\mathcal{O}(N^{-2/3}\log N)$, provided that the target density is twice continuously differentiable with non-vanishing curvature and the acceptance-rejection sampler uses the driver sequence

$$\mathcal{K}_M = \{\boldsymbol{x}_j = (j\alpha, j\beta) \ \ mod \ \ 1 \text{ for } j = 1, \ldots, M\},$$

where α, β are real algebraic numbers such that $1, \alpha, \beta$ is a basis of a number field over $\mathbb{Q}$ of degree 3. For the driver sequence

$$\mathcal{F}_k = \{\boldsymbol{x}_j = (j/F_k, \{jF_{k-1}/F_k\}) \text{ for } j = 1, \ldots, F_k\},$$

where F_k is the k-th Fibonacci number, we can remove the log factor to improve the convergence rate to $\mathcal{O}(N^{-2/3})$, where again N is the number of samples we accepted.

We introduce a criterion for measuring the goodness of driver sequences. The proposed approach is numerically tested by calculating the star-discrepancy of samples generated for some target densities using $\mathcal{K}_M$ and $\mathcal{F}_k$ as driver sequences. These results confirm that achieving a convergence rate beyond $N^{-1/2}$ is possible in practice using $\mathcal{K}_M$ and $\mathcal{F}_k$ as driver sequences in the acceptance-rejection sampler.

The layout of the chapter is as follows. We present the main theoretical results in Section 5.2, followed by a discussion of a criterion of good driver sequences in Section 5.3 and numerical experiments in Section 5.4. The desired bounds are proved in Section 5.5.

5.2 Discrepancy bounds beyond $N^{-1/2}$

5.2.1 Motivation

In [92], see also Chapter 3, we proposed a deterministic acceptance-rejection sampler using low-discrepancy point sets as driver sequences. Therein we proved that the star-discrepancy is of order $N^{-1/s}$ for target density functions defined in the $(s-1)$-dimensional cube, using (t, m, s)-nets as driver sequences. However, numerical results suggested a much better rate of convergence. Additionally, we proved a lower bound on the star-discrepancy with respect to a concave density function. The lower bound suggests a convergence rate of the form $N^{-\frac{2}{s+1}}$ for density functions defined in $[0,1]^{s-1}$, see Theorem 3.2.4 for details.

It is natural to ask whether the above bound is achievable, i.e., can we construct a driver sequence which yields a convergence rate of (almost) $N^{-2/3}$ in dimension 1 (note that dimension 1 corresponds to $s = 2$ in Theorem 3.2.4). In this chapter we present two types of constructions of driver sequences which yield a star-discrepancy of order (almost) $N^{-2/3}$ in one dimension. Here we present two types of constructions of driver sequences for which this property holds for the class of twice continuously

differentiable target densities with non-vanishing curvature. It uses the notions of non-vanishing curvature and number fields of degree 3, which we explain in the following.

The curvature of a twice continuously differentiable plane curve $\gamma(t) = (x(t), y(t))$ used in this paper is defined as

$$\kappa(t) = \frac{x'(t)y''(t) - y'(t)x''(t)}{((x'(t))^2 + (y'(t))^2)^{3/2}},$$

where the parameterization is such that $(x'(t))^2 + (y'(t))^2 \neq 0$ for all t in the domain. If the curve is given by a function $\gamma(t) = (t, f(t))$, then this reduces to

$$\kappa(t) = \frac{f''(t)}{(1 + (f'(t))^2)^{3/2}}.$$

Recall that if f is concave, then $\kappa \leq 0$ and if f is convex then $\kappa \geq 0$. By the assumption that the curve is twice continuously differentiable we have that κ is continuous. The assumption that the curvature is non-vanishing implies therefore that $|\kappa(t)| \geq c > 0$ for all t in the domain, and by the continuity of t, κ is either positive or negative everywhere. In particular, if the curve is given by a function, this means that the function is either strictly concave or strictly convex everywhere.

For the construction of a suitable driver sequence we use algebraic number fields over the set of rational numbers $\mathbb{Q}$. An algebraic number field over $\mathbb{Q}$ is a finite degree field extension of the field $\mathbb{Q}$ of rational numbers and its dimension as a vector space over $\mathbb{Q}$ is called the degree of the number field. For instance, the set $\mathbb{Q}(\xi, \xi^2) = \{a + b\xi + c\xi^2 \mid a, b, c \in \mathbb{Q}\}$, where ξ is a real root of a third degree irreducible polynomial over $\mathbb{Z}$, is a (real) number field of degree 3. In this case, $\{1, \xi, \xi^2\}$ is a basis of the number field.

5.2.2 Upper bounds on the star-discrepancy

Since in this chapter we are working on constructing good samples for densities in one dimension, the following algorithm now is the generic form of the acceptance-rejection algorithm based on a deterministic driver sequence for a density function defined in $[0, 1]$.

Algorithm 5.2.1. *Given a target density $\psi : [0,1] \to \mathbb{R}_+$, assume that there exists a constant $L < \infty$ such that $\psi(\boldsymbol{x}) < L$ for all $\boldsymbol{x} \in D$. Let $A = \{\boldsymbol{x} \in [0,1]^2 : \psi(x_1) \geq Lx_2\}$.*

i) Generate a uniformly distributed point set $G_M = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_M\}$ in $[0,1]^2$.

ii) Use the acceptance-rejection method for the points G_M with respect to the density ψ, i.e. we accept the point $\boldsymbol{x}_n$ if $\boldsymbol{x}_n \in A$, otherwise reject. Let $Y_N^{(2)} = A \cap G_M = \{\boldsymbol{z}_0, \boldsymbol{z}_1, \ldots, \boldsymbol{z}_{N-1}\}$ be the accepted sample set in $[0,1]^2$.

iii) Project the points in $Y_N^{(2)}$ onto the first coordinate. Let $Y_N(G_M) = \{y_0, y_1, \ldots, y_{N-1}\}$ be the projections of the point set $Y_N^{(2)}$.

iv) Return the point set $Y_N(G_M)$.

We estimate the star-discrepancy of samples generated by the acceptance-rejection algorithm for different driver sequences. For the driver sequence $\mathcal{K}_M$, we prove the following upper bound.

Theorem 5.2.2. *Let an unnormalized concave density function $\psi : [0,1] \to \mathbb{R}_+$ be twice continuously differentiable having non-vanishing curvature. Assume that there exists a constant $L < \infty$ such that $\psi(x) \leq L$ for all $x \in [0,1]$. Let*

$$\mathcal{K}_M = \{\boldsymbol{x}_j = (j\alpha, j\beta) \mod 1 \text{ for } j = 1, \ldots, M\},$$

where α, β are real algebraic numbers such that $1, \alpha, \beta$ is a basis of a number field over $\mathbb{Q}$ of degree 3. Then the discrepancy of $Y_N(\mathcal{K}_M) = \{y_0, y_1, \ldots, y_{N-1}\} \subseteq [0,1]$, generated by the acceptance-rejection sampler using $\mathcal{K}_M$ as driver sequence satisfies

$$D^*_{N,\psi}(Y_N(\mathcal{K}_M)) \leq C_\psi N^{-2/3} \log N,$$

where $N = |Y_N(\mathcal{K}_M)|$ is the number of points we accepted, and C_ψ is a constant depending on the target density ψ and the choice of α, β.

The proof of this result is presented in Section 5.5.1. This is an open-type construction, i.e. we can keep proposing new samples until a certain number of

points is accepted without changing the generated samples. In other words, the point set does not depends on the number of points. Compared with the open-type construction, closed-type constructions usually yield a better discrepancy bound in quasi-Monte Carlo methods. We also prove the following result which improves the previous bound by a factor of $\log N$. Before we can state this result, we introduce the following notation. Let F_k denote the k-th Fibonacci number given by

$$F_1 = F_2 = 1, F_k = F_{k-1} + F_{k-2} \text{ for } k \geq 3.$$

Let

$$\{x\} = x - \lfloor x \rfloor$$

denote the fractional part of the non-negative real number x.

Theorem 5.2.3. *Let an unnormalized concave density function $\psi : [0,1] \to \mathbb{R}_+$ be twice continuously differentiable having non-vanishing curvature. Assume that there exists a constant $L < \infty$ such that $\psi(x) \leq L$ for all $x \in [0,1]$. Let*

$$\mathcal{F}_k = \Big\{ \boldsymbol{x}_j = \big(\frac{j}{F_k}, \big\{\frac{jF_{k-1}}{F_k}\big\}\big) \text{ for } j = 1, \ldots, F_k \Big\}.$$

Then the discrepancy of $Y_N(\mathcal{F}_k) = \{y_0, y_1, \ldots, y_{N-1}\} \subseteq [0,1]$, generated by the acceptance-rejection sampler using $\mathcal{F}_k$ as driver sequence, satisfies

$$D^*_{N,\psi}(Y_N(\mathcal{F}_k)) \leq C'_\psi N^{-2/3},$$

where $N = |Y_N(\mathcal{F}_k)|$ is the number of points we accepted, and C'_ψ is a constant depending only on the target density ψ.

The proof of Theorem 5.2.3 follows by a similar argument as Theorem 5.2.2, with an additional estimation of a criterion of Fibonacci point sets (see Equation (5.3.1)) as discussed in Section 5.5.3.

In the driver sequence $\mathcal{F}_k$, the first component is evenly spaced and the second one is filled by taking the fractional part of jF_{k-1}/F_k. We can see that the construction relies on the k-th Fibonacci number F_k. Changing the number of points will provide a completely new point set. Thus $\mathcal{F}_k$ is a closed-type construction.

Lattice point sets of the form $\{(\frac{j}{N}, \{j\frac{g}{N}\}), j = 1, 2, \ldots, N\}$ have small star-discrepancy with respect to rectangular boxes if the coefficients in the continued fraction expansion of $\frac{g}{N}$ are bounded independently of N, see [60, Theorem 5.17]. In particular, for Fibonacci lattice point sets these coefficients are always 1. Niederreiter [58] explicitly finds values of g for N of the form 2^ℓ, 3^ℓ, 5^ℓ, such that the continued fraction coefficients are at most 3 for 2^ℓ and 3^ℓ, and at most 4 for 5^ℓ. It is reasonable to suggest that similar results to Theorem 5.2.3 and Corollary 5.2.5 below can also be obtained for lattice point sets based on the results in [58].

5.2.3 Integration errors

In [2], Aistleitner and Dick proved a generalized Koksma-Hlawka inequality for arbitrary Borel measures which states that for any function having bounded variation in the sense of Hardy and Krause (abbreviated as V_{HK}), the integration error can be bounded by a product of the variation of the integrand function times the discrepancy of the quadrature points.

We follow the definition of the variation V_{HK} from [2, Section 2]. Let f be a function on $[0,1]^s$. Let $B = [\boldsymbol{a}, \boldsymbol{b}] \subseteq [0,1]^s$ where $\boldsymbol{a} = (a_1, a_2, \ldots, a_s)$ and $\boldsymbol{b} = (b_1, b_2, \ldots, b_s)$. Let $\Delta^{(s)}(f, B)$ be a difference operator depending on f and B given by

$$\Delta^{(s)}(f, B) = \sum_{j_1=0}^{1} \ldots \sum_{j_s=0}^{1} (-1)^{j_1+\ldots+j_s} f(b_1 + j_1(a_1 - b_1), \ldots, b_s + j_s(a_s - b_s)).$$

For $k = 1, \ldots, s$, let $0 = x_0^{(k)} < x_1^{(k)} < \ldots < x_{m_k}^{(k)} = 1$ and let $\left[x_l^{(k)}, x_{l+1}^{(k)}\right), l = 0, 1, \ldots, m_k$ be a partition of $[0,1]$ and let $\mathcal{P}$ be the partition of $[0,1]^s$ constructed by

$$\mathcal{P} = \left\{ \left[x_{l_1}^{(1)}, x_{l_1+1}^{(1)}\right) \times \cdots \times \left[x_{l_s}^{(s)}, x_{l_s+1}^{(s)}\right), l_k = 0, \ldots m_k - 1, k = 1, \ldots, s \right\}.$$

Then the variation of f on $[0,1]^s$ in the sense of Vitali is given by

$$V^s(f; [0,1]^s) = \sup_{\mathcal{P}} \sum_{A \in \mathcal{P}} |\Delta^{(s)}(f; A)|,$$

where the supremum is extended over all partitions of $[0,1]^s$ into axis-parallel boxes generated by s one-dimensional partitions of $[0,1]$, as defined in $\mathcal{P}$. For $1 \le k \le s$ and $1 \le i_1 < \cdots < i_k \le s$, let $V^{(k)}(f; i_1, \cdots, i_k; [0,1]^s)$ denote the k-dimensional variation in the sense of Vitali of the restriction of f to the face

$$U_s^{(i_1,\cdots,i_k)} = \{(x_1, \cdots, x_s) \in [0,1]^s : x_j = 1 \text{ for all } j \neq i_1, \cdots, i_k\}$$

of $[0,1]^s$. Then the variation of f on $[0,1]^s$ in the sense of Hardy and Krause anchored at $\mathbf{1}$, abbreviated by V_{HK}, is given by

$$V_{HK}(f, [0,1]^s) = \sum_{d=1}^{s} \sum_{1 \le i_1 < \cdots < i_k \le s} V^k(f; i_1, \cdots, i_k; [0,1]^s).$$

With the above definition of V_{HK}, the corresponding Koksma-Hlawka type inequality with respect to a normalized Borel measure is given as follows.

Proposition 5.2.4. *Let f be a measurable function on $[0,1]^s$ which has bounded variation in the sense of Hardy and Krause, $V_{HK}(f) < \infty$. Let μ be a normalized Borel measure on $[0,1]^s$, and let $P_N = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ be a point set in $[0,1]^s$. Then*

$$\left| \frac{1}{N} \sum_{n=1}^{N} f(\boldsymbol{x}_n) - \int_{[0,1]^s} f(x) \, \mathrm{d}\mu(x) \right| \le V_{HK}(f) D^*_{N,\mu}(P_N).$$

In the following we use this result for dimension $s = 1$. In this case, if the function f is absolutely continuous, then the variation in the sense of Hardy and Krause can be written as $V_{HK}(f) = \int_0^1 |f'(x)| \, \mathrm{d}x$. Theorems 5.2.2 and 5.2.3 and Proposition 5.2.4 imply the following result.

Corollary 5.2.5. *Let $f : [0,1] \to \mathbb{R}$ have bounded variation $V_{HK}(f) < \infty$. Let ψ be non-negative, concave and twice continuously differentiable having non-vanishing curvature. Let $Y_N(\mathcal{K}_M)$ and $Y_N(\mathcal{F}_k)$ be the point set generated by the acceptance-rejection sampler using $\mathcal{K}_M$ and $\mathcal{F}_k$ as driver sequences respectively. Then we have*

$$\left| \frac{1}{N} \sum_{n=1}^{N} f(\boldsymbol{x}_n) - \frac{1}{C} \int_0^1 f(x)\psi(x) \, \mathrm{d}x \right| \le \begin{cases} C_\psi V_{HK}(f) N^{-2/3} \log N, & \text{for } Y_N(\mathcal{K}_M), \\ C'_\psi V_{HK}(f) N^{-2/3}, & \text{for } Y_N(\mathcal{F}_k), \end{cases}$$

where $N = |Y_N(\mathcal{K}_M)|, |Y_N(\mathcal{F}_k)|$ is the number of points we accepted, $C = \int_{[0,1]} \psi(x) \, \mathrm{d}x > 0$ and where C_ψ and C'_ψ are constants depending on ψ.

5.3 A quality criterion for driver sequences

In acceptance-rejection sampling, the choice of driver sequence can have a significant impact on the properties of the accepted samples. In this section, we will present a criterion which can be used to measure the quality of driver sequences.

Let $\boldsymbol{n} = (n_1, n_2) \in \mathbb{Z}^2$ and let $|\boldsymbol{n}| = \max\{|n_1|, |n_2|\}$. For a collection of points $Y_N = \{\boldsymbol{x}_j, j = 1, \ldots, N\}$ and $R > 0$, define the following quantity $\mathcal{Q}_R$ with respect to Y_N as follows.

$$\mathcal{Q}_R(Y_N) = \frac{1}{R} + \sum_{\substack{0<|\boldsymbol{n}|<R \\ \boldsymbol{n}\in\mathbb{Z}^2\setminus\boldsymbol{0}}} \Big(\frac{1}{|\boldsymbol{n}|^{3/2}} + \frac{1}{(1+|n_1|)(1+|n_2|)}\Big)\Big|\frac{1}{N}\sum_{j=1}^{N} e^{2\pi \mathrm{i}\boldsymbol{n}\cdot\boldsymbol{x}_j}\Big|. \quad (5.3.1)$$

The general Erdős-Turán inequality [11, Theorem 3] provides an upper bound on the discrepancy. We restate this result as a proposition in the following.

Proposition 5.3.1. *There exists a positive function $\phi(u)$ on $[0, \infty)$ with rapid decay at infinity such that for every collection of points $\{\boldsymbol{x}_j, j = 1, \ldots, N\} \subseteq \mathbb{R}^s$, for every bounded Borel set $\Omega \subset \mathbb{R}^s$, and for every $R > 0$,*

$$\begin{aligned} &\Big|\frac{1}{N}\sum_{j=1}^{N}\sum_{\boldsymbol{m}\in\mathbb{Z}^2} 1_\Omega(\boldsymbol{x}_j + \boldsymbol{m}) - \lambda(\Omega)\Big| \\ \leq\ & |\hat{H}_R(0)| + \sum_{\substack{\boldsymbol{n}\in\mathbb{Z}^2 \\ 0<|\boldsymbol{n}|<R}} (|\hat{1}_D(\boldsymbol{n})| + |\hat{H}_R(n)|)\Big|\frac{1}{N}\sum_{j=1}^{N} e^{2\pi \mathrm{i}\boldsymbol{n}\cdot\boldsymbol{x}_j}\Big|, \end{aligned}$$

where $H_R(x) = \phi(R\,\mathrm{dist}(x, \partial\Omega))$ with dist *is the Euclidean distance in $\mathbb{R}^s$, $\hat{H}_R(0)$ is the zeroth Fourier coefficient of H_R and $\hat{1}_\Omega$ is the Fourier transform of the indicator function along the boundary of Ω.*

Remark. *Note that in [11] they define the positive function ϕ as follows. Let $\kappa(\xi)$ be a smooth radial function supported in $\{\xi \in \mathbb{R}^2 : |\xi| < 1/2, \int_{\mathbb{R}^2} \kappa^2(\xi)\,\mathrm{d}\xi = 1\}$ and let*

$$\begin{aligned} K(x) &= \int_{\mathbb{R}^2} (1+|\xi|^2)^{-3/2} (\kappa * \kappa)(\xi) e^{2\pi \mathrm{i}\xi\cdot x}\,\mathrm{d}\xi, \\ \phi(u) &= e^{2\pi}\Big(\int_{|y|\leq 1} K(y)\,\mathrm{d}y\Big)^{-1} \int_{\{|y|\geq u\}} K(y)\,\mathrm{d}y, \end{aligned}$$

where $*$ is the convolution operator.

Under certain smooth conditions on the boundary curve of Ω, the quantity criterion $\mathcal{Q}_R$ can be derived from the right side of Erdős-Turán inequality by working out the corresponding Fourier coefficient decay. More precisely, if the boundary curve of Ω is twice continuously differentiable having non-vanishing curvature, then we have the formula for $\mathcal{Q}_R$ as shown in Equation 5.3.1.

The following theorem shows a connection between the criterion $\mathcal{Q}_R$ for the driver sequence and the star-discrepancy of the samples obtained by the acceptance-rejection algorithm using a deterministic driver sequence. In the following discussion, the notation $x_N \lesssim y_N$ means that there exists a positive constant θ such that $x_N \leq \theta y_N$ for all N.

Theorem 5.3.2. *Let the unnormalized concave density function $\psi : [0,1] \to \mathbb{R}_+$ be twice continuously differentiable having non-vanishing curvature. Assume that there exists a constant $L < \infty$ such that $\psi(x) \leq L$ for all $x \in [0,1]$. Let $Y_N(G_M) = \{y_0, y_1, \ldots, y_{N-1}\} \subseteq [0,1]$ be generated by the acceptance-rejection sampler using the point set G_M of cardinality M as the driver sequence. Then we have*

$$D^*_{N,\psi}(Y_N(G_M)) \lesssim \mathcal{Q}_R(G_M).$$

The proof of Theorem 5.5.2 is presented in Section 5.5.2.

5.4 Numerical experiments

To demonstrate the performance of the deterministic acceptance-rejection samplers, we consider two density functions defined on $[0,1]$ and calculate the star-discrepancy of the samples generated by the proposed methods. For comparison purpose, the convergence rate of the original algorithm using random points and regular grids as driver sequence are also presented. Note that numerical results are presented in a log-log scale.

Example 5.4.1. *Let the target density* $\psi : [0,1] \to \mathbb{R}^+$ *be given by*

$$\psi(x) = \frac{3}{16}\left(4\sin\left(\frac{\pi x}{2}\right) - x^{5/2} - x^2\right).$$

This density function satisfies all smoothness conditions in our theory. The numerical results shown in Figure 5.1 suggest an empirical convergence rate of approximately $N^{-0.75}$ for samples of ψ obtained by the deterministic acceptance-rejection sampler using the driver sequence

$$\mathcal{K}_M = \{\boldsymbol{x}_j = (j\alpha, j\beta) \mod 1 \text{ for } j = 1, \ldots, M\}.$$

In the test we choose the real root of the polynomial x^3+2x+2. Eisenstein's criterion implies that this polynomial is irreducible over $\mathbb{Z}$. The root ξ is approximated by -0.770916997059248 and we set $\alpha = \xi$ and $\beta = \xi^2$.

Similarly, using the Fibonacci lattice point set

$$\mathcal{F}_k = \{\boldsymbol{x}_j = (j/F_k, \{jF_{k-1}/F_k\}) \text{ for } j = 1, \ldots, F_k\},$$

the numerical experiments show a convergence rate of approximately $N^{-0.8}$. The original acceptance-rejection sampler in the random setting produced samples whose star-discrepancy converges at roughly $N^{-1/2}$. A similar result is observed for the regular grid B_M given by

$$B_M = \left\{\left(\frac{j}{\lfloor\sqrt{M}\rfloor}, \frac{m}{\lfloor\sqrt{M}\rfloor}\right) \mid j, m = 1, \ldots, \lfloor\sqrt{M}\rfloor\right\}.$$

It is worth noticing that Fibonacci lattice points always provided the smallest value of the discrepancy. The acceptance rate is roughly 69% for the first example.

Example 5.4.2. *Consider the twice continuously differentiable and strictly convex target density function*

$$\psi(x) = \begin{cases} -\frac{1}{2}x^4 - \frac{1}{6}x^2 + \frac{107}{108}, & x \in [0, \frac{1}{3}), \\ -\frac{3}{4}x^4 - \frac{2}{27}x + 1, & x \in [\frac{1}{3}, 1]. \end{cases}$$

We again observe much better results with deterministic driver sequences, $\mathcal{F}_k$ and $\mathcal{K}_M$, compared with pseudo-random points and regular grids as shown in Figure 5.2. As observed in the first example, a Fibonacci lattice point set $\mathcal{F}_k$ yields a

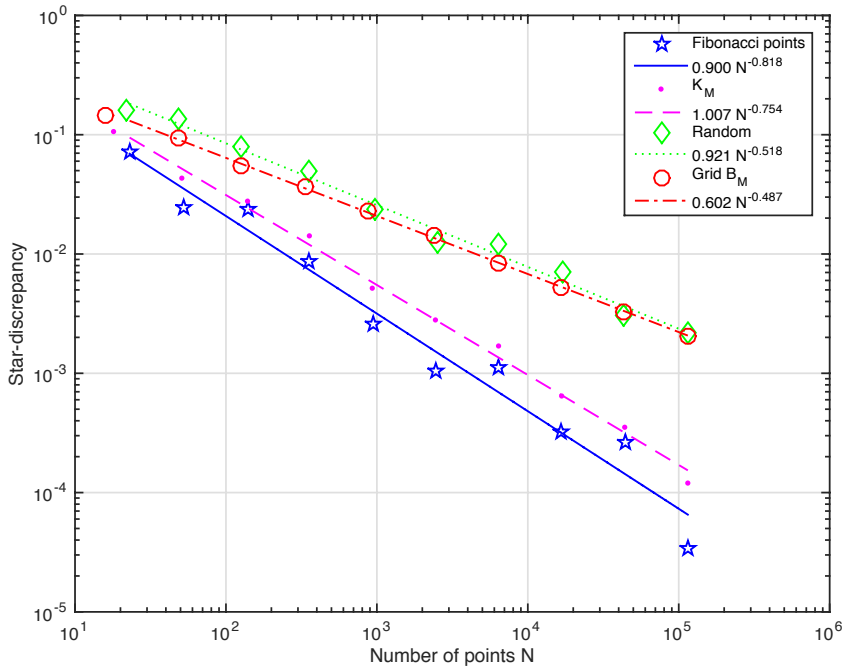


Figure 5.1: Convergence order of the star-discrepancy with respect to different driver sequences for Example 5.4.1.

slightly better numerical result compared to the point set $\mathcal{K}_M$ in this experiment. The acceptance rate is around 80% for Example 5.4.2.

5.5 Proofs

5.5.1 Proof of Theorem 5.2.2

The proof of Theorem 5.2.2 is motivated by a recent paper due to Brandolini et al. [11]. Therein they proved an upper bound for the following discrepancy associated with a convex domain with smooth boundary. We recall the main results pertaining to our discussion here.

Let Ω be a bounded convex domain in $\mathbb{R}^2$ such that the boundary curve is twice continuously differentiable having non-vanishing curvature. For $\boldsymbol{t} = (t_1, t_2) \in (0,1)^2$

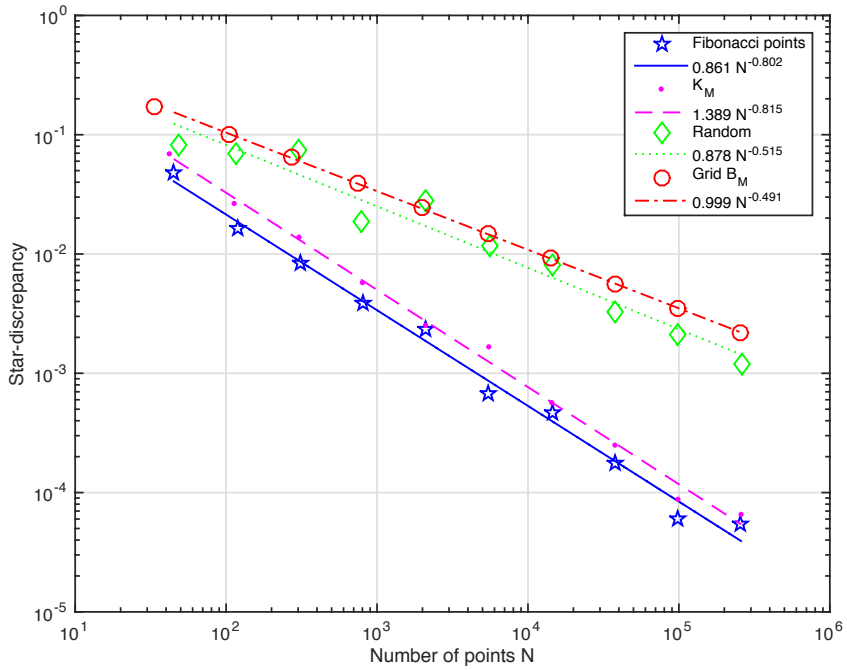


Figure 5.2: Convergence order of the star-discrepancy with respect to different driver sequences for Example 5.4.2.

and any $\boldsymbol{x} \in \mathbb{R}^2$, let

$$I(\boldsymbol{t}, \boldsymbol{x}) = \bigcup_{\boldsymbol{m} \in \mathbb{Z}^2} ([0, t_1] \times [0, t_2] + \boldsymbol{x} + \boldsymbol{m}).$$

Consider the following discrepancy defined with respect to the set Ω and a point set $P_N = \{\boldsymbol{x}_j, j = 1, \ldots, N\}$ in $\mathbb{R}^2$,

$$D_N^*(P_N, \Omega) = \sup_{\substack{\boldsymbol{t} \in [0,1]^2 \\ \boldsymbol{x} \in \mathbb{R}^2}} \left| \frac{1}{N} \sum_{j=1}^{N} \sum_{\boldsymbol{m} \in \mathbb{Z}^2} 1_{I(\boldsymbol{t}, \boldsymbol{x}) \cap \Omega}(\boldsymbol{x}_j + \boldsymbol{m}) - \lambda(I(\boldsymbol{t}, \boldsymbol{x}) \cap \Omega) \right|, \quad (5.5.1)$$

where λ denotes the Lebesgue measure.

The following result is [11, Theorem 2], which plays a crucial role in the proof of Theorem 5.2.2.

Proposition 5.5.1. *Suppose that Ω is a convex domain in $\mathbb{R}^2$ such that the boundary curve is twice continuously differentiable having non-vanishing curvature. Let $1, \alpha, \beta$*

be a basis of a number field over $\mathbb{Q}$ *of degree* 3. *Let*

$$\mathcal{K}_N = \{\boldsymbol{x}_j = (j\alpha, j\beta) \text{ for } j = 1, \dots, N\}.$$

For the discrepancy defined in Equation (5.5.1), *we have*

$$D_N^*(P_N, \Omega) \leq cN^{-2/3} \log N,$$

where the constant c *depends on the minimum and maximum of the curvature of the boundary of* Ω *and the length of the boundary, and on the numbers* α *and* β.

The proof of [11, Theorem 2] actually shows that a slightly more general statement holds, which we describe in the following.

For given $\boldsymbol{t}$ and $\boldsymbol{x}$, the set $I(\boldsymbol{t}, \boldsymbol{x})$ is the union of infinitely many rectangles of the form $[0, t_1] \times [0, t_2] + \boldsymbol{x} + \boldsymbol{m}$, where $\boldsymbol{m} \in \mathbb{Z}^2$. Let $K_1, \dots, K_q$ denote all those rectangles which have non-empty intersection with Ω, i.e., $K_r = [0, t_1] \times [0, t_2] + \boldsymbol{x} + \boldsymbol{m}_r$ for suitable choices of $\boldsymbol{m}_r \in \mathbb{Z}^2$ with $K_r \cap \Omega \neq \emptyset$. Then

$$\begin{aligned} &\frac{1}{N} \sum_{j=1}^{N} \sum_{\boldsymbol{m} \in \mathbb{Z}^2} 1_{I(\boldsymbol{t}, \boldsymbol{x}) \cap \Omega}(\boldsymbol{x}_j + \boldsymbol{m}) - \lambda(I(\boldsymbol{t}, \boldsymbol{x}) \cap \Omega) \\ &= \sum_{r=1}^{q} \left(\frac{1}{N} \sum_{j=1}^{N} \sum_{\boldsymbol{m} \in \mathbb{Z}^2} 1_{K_r \cap \Omega}(\boldsymbol{x}_j + \boldsymbol{m}) - \lambda(K_r \cap \Omega) \right). \end{aligned} \tag{5.5.2}$$

In [11, pp. 10] the authors state that they prove their result by showing the upper bound for a single piece K_r, i.e. they show the bound

$$\sup_{\substack{\boldsymbol{t} \in [0,1]^2 \\ \boldsymbol{x} \in \mathbb{R}^2}} \left| \frac{1}{N} \sum_{j=1}^{N} \sum_{\boldsymbol{m} \in \mathbb{Z}^2} 1_{K_r \cap \Omega}(\boldsymbol{x}_j + \boldsymbol{m}) - \lambda(K_r \cap \Omega) \right| \leq c_s' N^{-2/3} \log N. \tag{5.5.3}$$

The bound on $D_N^*(\mathcal{K}, \Omega)$ then follows by the triangle inequality. We use (5.5.3) rather than Proposition 5.5.1 in the following.

Note that we are only interested in sets K_r which are contained in the unit square, i.e. $K_r \subset [0, 1]^2$. In this case we have

$$\frac{1}{N} \sum_{j=1}^{N} \sum_{\boldsymbol{m} \in \mathbb{Z}^2} 1_{K_r \cap \Omega}(\boldsymbol{x}_j + \boldsymbol{m}) = \frac{1}{N} \sum_{j=1}^{N} 1_{K_r \cap \Omega}(\boldsymbol{x}_j \pmod 1),$$

for any point set $\{\boldsymbol{x}_1 \ldots, \boldsymbol{x}_N\} \subset \mathbb{R}^2$. Thus we obtain from (5.5.3) that

$$\sup_{\boldsymbol{t}\in[0,1]^2} \left| \frac{1}{N} \sum_{j=1}^{N} 1_{[\boldsymbol{0},\boldsymbol{t}]\cap\Omega}(\boldsymbol{x}_j \pmod 1) - \lambda([\boldsymbol{0},\boldsymbol{t}] \cap \Omega) \right| \leq c_s' N^{-2/3} \log N. \tag{5.5.4}$$

In order to be able apply this result in our setting, it remains to construct a suitable convex set Ω in $[0,1]^2$ which has the graph of ψL^{-1} as part of its boundary. We define the boundary of the set Ω by extending the graph of ψL^{-1} using a Bézier curve such that the curve is twice continuously differentiable. The Bézier curve can be constructed using the derivative information of ψL^{-1} at the boundary and further control points to control the curvature of the curve. The set Ω enclosed by this curve then satisfies the assumptions that its boundary is twice continuously differentiable with non-vanishing curvature. The details of the construction are left to the reader (see [27, Chapter 6]).

With these settings, the desired discrepancy bound in Theorem 5.2.2 now follows from (5.5.4).

5.5.2 Proof of Theorem 5.3.2

Proof of Theorem 5.3.2. By the definition of the star-discrepancy with respect to a density function, we have

$$D^*_{N,\psi}(Y_N(G_M)) = \sup_{t\in[0,1]} \left| \frac{1}{N} \sum_{j=0}^{N-1} 1_{[0,t)}(y_j) - \frac{1}{C} \int_{[0,t)} \psi(z)\,\mathrm{d}z \right|.$$

Let $A = \{\boldsymbol{x} = (x_1, x_2) \in [0,1]^2 : \psi(x_1) \geq L x_2\}$ and $J_t^* = ([0,t) \times [0,1)) \bigcap A$ for $t \in [0,1]$.

Algorithm 5.2.1 implies that the points $y_1, \ldots, y_N$ are the first coordinates of the points of the driver sequence $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_M$ which are in the set A. Hence we have

$$\sum_{j=1}^{M} 1_{J_t^*}(\boldsymbol{x}_j) = \sum_{j=1}^{N} 1_{[0,t)}(y_j).$$

Note that $C = \int_0^1 \psi(z)\,\mathrm{d}z = L\lambda(A)$ and for any $t \in [0,1]$ we have $\int_0^t \psi(z)\,\mathrm{d}z = L\lambda(J_t^*)$. Therefore,

$$\begin{aligned}
&\Big|\frac{1}{N}\sum_{j=1}^{N} 1_{[0,t)}(y_j) - \frac{1}{C}\int_{[0,t)} \psi(z)\,\mathrm{d}z\Big| \\
= \;& \Big|\frac{1}{N}\sum_{j=1}^{M} 1_{J_t^*}(\boldsymbol{x}_j) - \frac{1}{\lambda(A)}\lambda(J_t^*)\Big| \\
\le \;& \frac{M}{N}\Big|\frac{1}{M}\sum_{j=1}^{M} 1_{J_t^*}(\boldsymbol{x}_j) - \lambda(J_t^*)\Big| + \Big|\lambda(J_t^*)\Big(\frac{M}{N} - \frac{1}{\lambda(A)}\Big)\Big| \\
\le \;& \frac{M}{N}\Big(\Big|\frac{1}{M}\sum_{j=1}^{M} 1_{J_t^*}(\boldsymbol{x}_j) - \lambda(J_t^*)\Big| + \Big|\lambda(A)\Big(1 - \frac{1}{\lambda(A)}\frac{N}{M}\Big)\Big|\Big) \\
\le \;& \frac{M}{N}\Big(\Big|\frac{1}{M}\sum_{j=1}^{M} 1_{J_t^*}(\boldsymbol{x}_j) - \lambda(J_t^*)\Big| + \Big|\lambda(A) - \frac{1}{M}\sum_{j=1}^{M} 1_{J_A}(\boldsymbol{x}_j)\Big|\Big) \\
\le \;& \frac{2M}{N}\sup_{t\in[0,1]}\Big|\frac{1}{M}\sum_{j=1}^{M} 1_{J_t^*}(\boldsymbol{x}_j) - \lambda(J_t^*)\Big|, \qquad (5.5.5)
\end{aligned}$$

where we used the estimation $\lambda(J_t^*) \le \lambda(A)$ and the fact that $N = \sum_{j=1}^{M} 1_A(\boldsymbol{x}_j)$ is the number of accepted points.

For the Borel set $J_t^* \subset [0,1)^2$ we have

$$\frac{1}{M}\sum_{j=1}^{M}\sum_{\boldsymbol{m}\in\mathbb{Z}^2} 1_{J_t^*}(\boldsymbol{x}_j + \boldsymbol{m}) = \frac{1}{M}\sum_{j=1}^{M} 1_{J_t^*}(\boldsymbol{x}_j \pmod 1).$$

Then by the general Erdős-Turán inequality in Proposition 5.3.1, we obtain, for every $R > 0$,

$$\Big|\frac{1}{M}\sum_{j=1}^{M} 1_{J_t^*}(\boldsymbol{x}_j) - \lambda(J_t^*)\Big| \le |\hat{H}_R(0)| + \sum_{\substack{\boldsymbol{n}\in\mathbb{Z}^2\\ 0<|\boldsymbol{n}|<R}} (|\hat{1}_{J_t^*}(\boldsymbol{n})| + |\hat{H}_R(\boldsymbol{n})|)\Big|\frac{1}{M}\sum_{j=1}^{M} e^{2\pi \mathrm{i}\boldsymbol{n}\cdot\boldsymbol{x}_j}\Big|.$$

Note that J_t^* is the intersection of the convex set Ω whose boundary was constructed using a Bézier curve which is twice continuously differentiable with non-vanishing curvature (see the proof of Theorem 5.2.2), and the rectangle $[0,t)\times[0,1)$.

Thus we can use the following estimations from [11, Lemma 10 & Lemma 11],

$$\begin{aligned} |\hat{H}_R(0)| &\lesssim \frac{1}{R}, \\ |\hat{H}_R(\boldsymbol{n})| &\lesssim \frac{1}{|\boldsymbol{n}|^{3/2}} + \frac{1}{(1+|n_1|)(1+|n_2|)}, \\ |\hat{1}_{J_t^*}(\boldsymbol{n})| &\lesssim \frac{1}{|\boldsymbol{n}|^{3/2}} + \frac{1}{(1+|n_1|)(1+|n_2|)}, \end{aligned}$$

the result now follows. □

5.5.3 Proof of Theorem 5.2.3

Theorem 5.2.3 follows immediately from Theorem 5.3.2 and Lemma 5.5.2 below.

Lemma 5.5.2. *Let F_k denote the k-th Fibonacci number, given by $F_1 = 1, F_2 = 1$ and $F_k = F_{k-1} + F_{k-2}$ for $k \geq 3$. Let*

$$\mathcal{F}_k = \Big\{ \boldsymbol{x}_j = \big(\frac{j}{F_k}, \{\frac{jF_{k-1}}{F_k}\}\big) \text{ for } j = 1, \dots F_k \Big\},$$

where $\{x\}$ denotes the fractional part of a non-negative number x, more precisely, $\{x\} = x - \lfloor x \rfloor$. Then we have

$$\mathcal{Q}_R(\mathcal{F}_k) \lesssim F_k^{-2/3},$$

for $R = F_{\lceil 2k/3 \rceil}$. The implied constant is independent of F_k.

Proof. First we have

$$\begin{aligned} \Big| \frac{1}{F_k} \sum_{j=1}^{F_k} e^{2\pi i \boldsymbol{n} \cdot \left(\frac{j}{F_k}, \frac{jF_{k-1}}{F_k}\right)} \Big| &= \Big| \frac{1}{F_k} \sum_{j=1}^{F_k} \big(e^{2\pi i n \cdot (1, F_{k-1})/F_k}\big)^j \Big| \\ &= \begin{cases} 1, & \text{if } F_k | (n_1 + n_2 F_{k-1}), \\ 0, & \text{if } F_k \nmid (n_1 + n_2 F_{k-1}), \end{cases} \end{aligned}$$

where $F_k|(n_1+n_2F_{k-1})$ means that F_k divides $(n_1+n_2F_{k-1})$, which implies that there is an $\ell\in\mathbb{Z}$ such that $n_1+n_2F_{k-1}=\ell F_k$. Hence

$$\begin{aligned}&\sum_{\substack{\boldsymbol{n}\in\mathbb{Z}^2\\0<|\boldsymbol{n}|<R}}\Big(\frac{1}{|\boldsymbol{n}|^{3/2}}+\frac{1}{(1+|n_1|)(1+|n_2|)}\Big)\Big|\frac{1}{F_k}\sum_{j=1}^{F_k}e^{2\pi i n\cdot\left(\frac{j}{F_k},\frac{jF_{k-1}}{F_k}\right)}\Big|\\ =&\sum_{\substack{\boldsymbol{n}\in\mathbb{Z}^2\\0<|\boldsymbol{n}|<R\\F_k|(n_1+n_2F_{k-1})}}\Big(\frac{1}{|\boldsymbol{n}|^{3/2}}+\frac{1}{(1+|n_1|)(1+|n_2|)}\Big).\end{aligned}\tag{5.5.6}$$

From [60, Definition 5.4 & Equation (5.11) & Theorem 5.17] we obtain that

$$\sum_{\boldsymbol{n}}\frac{1}{\max\{1,|n_1|\}\max\{1,|n_2|\}}\lesssim\frac{(\log F_k)^2}{F_k},$$

where the sum is over all $\boldsymbol{n}=(n_1,n_2)\neq(0,0)$ with $n_1+n_2F_{k-1}\equiv 0 \pmod{F_k}$ and $-F_k/2<n_i\leq F_k/2$ for $i=1,2$. Hence

$$\begin{aligned}\sum_{\substack{0<|\boldsymbol{n}|<R\\F_k|(n_1+n_2F_{k-1})}}\frac{1}{(1+|n_1|)(1+|n_2|)}&\leq\sum_{\substack{0<|\boldsymbol{n}|<R\\F_k|(n_1+n_2F_{k-1})}}\frac{1}{\max\{1,|n_1|\}\max\{1,|n_2|\}}\\&\lesssim\frac{(\log F_k)^2}{F_k}.\end{aligned}$$

Note that if $n_1=0$, then $F_k|n_2F_{k-1}$ which implies $F_k|n_2$ since $\gcd(F_k,F_{k-1})=1$. It further implies $n_2=0$ by realising that $|n_2|\leq R=F_{\lceil 2k/3\rceil}<F_k$ for $k\geq 3$.

If $n_2=0$, then $F_k|n_1$, which implies that $n_1=0$ since $|n_1|\leq R=F_{\lceil 2k/3\rceil}<F_k$ for $k\geq 3$.

Since $F_k|(n_1+n_2F_{k-1})$, there is an $\ell\in\mathbb{Z}$ such that $n_1+n_2F_{k-1}=\ell F_k$. For given n_2, there is at most one value $\ell\in\mathbb{Z}$ such that $-R<n_1=\ell F_k-n_2F_{k-1}<R$.

Now we estimate the remaining term of Equation (5.5.6). We have

$$\sum_{\substack{0<|\boldsymbol{n}|<R\\F_k|(n_1+n_2F_{k-1})}}\frac{1}{|\boldsymbol{n}|^{3/2}}=\sum_{\substack{-R<n_2<R\\n_2\neq 0}}\sum_{\substack{\ell\in\mathbb{Z}\\-R<\ell F_k-n_2F_{k-1}<R}}\frac{1}{\max\{|n_2|,|\ell F_k-n_2F_{k-1}|\}^{\frac{3}{2}}}.\tag{5.5.7}$$

To bound this term we need some preliminary results on Fibonacci lattice point sets $\mathcal{F}_k$. The star-discrepancy with respect to uniform distribution of the Fibonacci

point set $\mathcal{F}_k$ is bounded by

$$D^*_{F_k}(\mathcal{F}_k) \leq c_0 \frac{\log F_k}{F_k},$$

see [60, pp. 124]. The star-discrepancy $D^*_{F_k}(\mathcal{F}_k)$ is defined with respect to rectangles $[\mathbf{0}, \boldsymbol{t}) = [0, t_1) \times [0, t_2)$ for all $(t_1, t_2) \in [0, 1]^2$. To switch to the discrepancy $D_{F_k}(\mathcal{F}_k)$ with respect to arbitrary rectangles $[\boldsymbol{a}, \boldsymbol{b}) \subseteq [0, 1]^2$, we use the inequality $D_{F_k}(\mathcal{F}_k) \leq 4D^*_{F_k}(\mathcal{F}_k)$, see [60, Proposition 2.4].

Consider a rectangle V of the following form,

$$V = \Big[\frac{a}{F_k}, \frac{a+u}{F_k}\Big) \times \Big[\frac{b}{F_k}, \frac{b+v}{F_k}\Big).$$

By the definition of the star-discrepancy, it follows that

$$\Big|\frac{|V \cap \mathcal{F}_k|}{F_k} - \frac{uv}{F_k^2}\Big| \leq D_{F_k}(\mathcal{F}_k) \leq 4D^*_{F_k}(\mathcal{F}_k) \leq 4c_0 \frac{\log F_k}{F_k}.$$

This implies that

$$|V \cap \mathcal{F}_k| \leq 4c_0 \log F_k + \frac{uv}{F_k}. \tag{5.5.8}$$

We now consider the double sum in Equation (5.5.7). We divide the range of $0 < |n_2| < F_{\lceil 2k/3 \rceil}$ into

$$F_i \leq |n_2| < F_{i+1} \text{ for } i = 2, 3, \ldots, \Big\lceil \frac{2k}{3} \Big\rceil - 1.$$

Let $a = F_i$ and $u = F_{i-1}$, then $a + u = F_{i+1}$. Similarly we divide the range of $0 < |n_1| = |\ell F_k - n_2 F_{k-1}| < F_{\lceil 2k/3 \rceil}$ into

$$F_m \leq |n_1| < F_{m+1} \text{ for } m = 2, 3, \ldots, \Big\lceil \frac{2k}{3} \Big\rceil - 1.$$

Let $b = F_m$ and $v = F_{m-1}$, then $b + v = F_{m+1}$. With those settings we have

$$\begin{aligned} \frac{a}{F_k} \leq \frac{|n_2|}{F_k} < \frac{a+u}{F_k}, \\ \frac{b}{F_k} \leq \Big|\frac{n_2 F_{k-1}}{F_k} - \ell\Big| < \frac{b+v}{F_k}. \end{aligned}$$

By Equation (5.5.8), the number of Fibonacci points in the rectangle V, given by $|\mathcal{F}_k \cap V|$, is therefore bounded by $4c_0 \log F_k + \frac{F_{i-1}F_{m-1}}{F_k}$. This is equivalent to the

statement that the number of (n_1, n_2) with $n_1 = \ell F_k - n_2 F_{k-1}$, $a = F_i \le |n_2| < F_{i+1} = a + u$, and $b = F_m \le |n_1| < F_{m+1} = b + v$ is bounded above by a constant (which is independent of i, k, m) times

$$4c_0 \log F_k + \frac{F_{i-1} F_{m-1}}{F_k}. \tag{5.5.9}$$

This result can be obtained by considering the following four cases,

(i) $a \le n_2 < a + u$ and $b \le n_2 F_{k-1} - \ell F_k < b + v$,

(ii) $a \le -n_2 < a + u$ and $b \le -(n_2 F_{k-1} - \ell F_k) < b + v$,

(iii) $a \le n_2 < a + u$ and $b \le -(n_2 F_{k-1} - \ell F_k) < b + v$,

(iv) $a \le -n_2 < a + u$ and $b \le n_2 F_{k-1} - \ell F_k < b + v$.

More precisely, for case (iii) and (iv), we consider the point set

$$\begin{aligned} \mathcal{F}'_k &= \Big\{ \big(\frac{j}{F_k}, \{ -\frac{j F_{k-1}}{F_k} \} \big) \mid j = 1, \dots F_k \Big\} \\ &= \Big\{ \big(\frac{j}{F_k}, 1 - \{ \frac{j F_{k-1}}{F_k} \} \big) \mid j = 1, \dots F_k \Big\}. \end{aligned}$$

Then the star-discrepancy of $\mathcal{F}'_k$, $D^*_{F_k}(\mathcal{F}'_k) \lesssim \frac{\log F_k}{F_k}$ by noting that $\boldsymbol{x}'_j$ is a reflection of $\boldsymbol{x}_j \in \mathcal{F}_k$ and the inequalities $D^*_{F_k}(\mathcal{F}_k) \le D_{F_k}(\mathcal{F}'_k) \le 4 D^*_{F_k}(\mathcal{F}'_k)$.

On the other hand, for all $1 \le n_2 < F_{i+1}$ and $k > i$, using the continued fractions technique mentioned in [60, Appendix B] and a property of Fibonacci numbers, we obtain

$$|n_1| = |\ell F_k - n_2 F_{k-1}| \ge |F_{i-1} F_k - F_i F_{k-1}| = F_{k-i}. \tag{5.5.10}$$

Since $|n_1| \le |\boldsymbol{n}| < R = F_{\lceil 2k/3 \rceil}$, there is no solution if $k - i \ge \lceil \frac{2k}{3} \rceil$, i.e. $i \le \lfloor \frac{k}{3} \rfloor$.

Therefore

$$\begin{aligned}
&\sum_{\substack{0<|\boldsymbol{n}|<R\\ \boldsymbol{n}\in\mathbb{Z}^2}} \frac{1}{|\boldsymbol{n}|^{3/2}}\\
&= \sum_{\substack{-R<n_2<R\\ n_2\neq 0}} \sum_{-R<\ell F_k-n_2F_{k-1}<R} \frac{1}{\max\{|n_2|,|\ell F_k-n_2F_{k-1}|\}^{3/2}}\\
&= 2\sum_{i=\lfloor k/3\rfloor+1}^{\lceil 2k/3\rceil-1}\sum_{n_2=F_i}^{F_{i+1}-1}\sum_{m=k-i}^{\lfloor 2k/3\rfloor-1} \sum_{F_m\le|\ell F_k-n_2F_{k-1}|<F_{m+1}} \frac{1}{(\max\{|n_2|,|\ell F_k-n_2F_{k-1}|\})^{3/2}},
\end{aligned} \tag{5.5.11}$$

where we used that for $(n_1,n_2)\in\mathbb{Z}^2$ which satisfy $0<\max\{|n_1|,|n_2|\}<R$ and $F_k|(n_1+n_2F_{k-1})$, also $(-n_1,-n_2)\in\mathbb{Z}^2$ satisfy these properties.

To further estimate the right-hand side of Equation (5.5.11), we use the following inequalities. For $F_i\le|n_2|<F_{i+1}$ and $F_m\le|n_1|<F_{m+1}$ we have

$$\max\{|n_2|,|\ell F_k-n_2F_{k-1}|\}\ge\max\{F_i,F_m\}.$$

For $\lfloor\frac{k}{3}\rfloor<i<\lceil\frac{k}{2}\rceil$ and $k-i\le m<k$, we have $\max\{F_i,F_m\}=F_m$.

Applying the bound given in (5.5.9) in each case, we obtain from Equation (5.5.11) that

$$\begin{aligned}
\sum_{\substack{0<|\boldsymbol{n}|<R\\ \boldsymbol{n}\in\mathbb{Z}^2}} \frac{1}{|\boldsymbol{n}|^{3/2}} \;\le\; & 2\sum_{i=\lfloor k/3\rfloor+1}^{\lceil k/2\rceil-1}\sum_{m=k-i}^{k}\Big(\frac{4c_0\log F_k}{F_m^{3/2}}+\frac{F_{i-1}F_{m-1}}{F_m^{3/2}F_k}\Big)\\
&+2\sum_{i=\lceil k/2\rceil}^{\lceil 2k/3\rceil-1}\sum_{m=k-i}^{\lfloor 2k/3\rfloor-1}\Big(\frac{4c_0\log F_k}{\max\{F_i,F_m\}^{\frac{3}{2}}}+\frac{F_{i-1}F_{m-1}}{\max\{F_i,F_m\}^{\frac{3}{2}}F_k}\Big).
\end{aligned}$$

It is well known that $F_i=[\varphi^i/\sqrt{5}]$ with $\varphi=(1+\sqrt{5})/2$, where $[\cdot]$ denotes the nearest integer function given by the integer $[x]=\gamma\in\mathbb{Z}$ which satisfies that

$\gamma - \frac{1}{2} < x \leq \gamma + \frac{1}{2}$. Thus we have

$$\begin{aligned}
\sum_{i=\lfloor k/3\rfloor+1}^{\lceil k/2\rceil-1} \sum_{m=k-i}^{\lfloor 2k/3\rfloor-1} \frac{\log F_k}{F_m^{3/2}} &\lesssim \log F_k \sum_{i=\lfloor k/3\rfloor+1}^{\lceil k/2\rceil-1} \sum_{m=k-i}^{\lfloor 2k/3\rfloor-1} \frac{1}{\varphi^{\frac{3}{2}m}} \\
&\lesssim \log F_k \sum_{i=\lfloor k/3\rfloor+1}^{\lceil k/2\rceil-1} \frac{\varphi^{-\frac{3}{2}(k-i)}\big(1-\varphi^{-\frac{3}{2}(i-k/3+1)}\big)}{1-\varphi^{-3/2}} \\
&\lesssim \frac{\log F_k}{\varphi^{\frac{3}{2}k}} \sum_{i=\lfloor k/3\rfloor+1}^{\lceil k/2\rceil-1} \varphi^{\frac{3}{2}i} \\
&\lesssim \frac{\log F_k}{\varphi^{\frac{3}{2}k}} \varphi^{\frac{3}{4}k} \lesssim \frac{\log F_k}{F_k^{3/4}}, \qquad (5.5.12)
\end{aligned}$$

and

$$\begin{aligned}
\sum_{i=\lfloor k/3\rfloor+1}^{\lceil k/2\rceil-1} \sum_{m=k-i}^{\lfloor 2k/3\rfloor-1} \frac{F_{i-1}F_{m-1}}{F_m^{3/2}F_k} &\lesssim \sum_{i=\lfloor k/3\rfloor+1}^{\lceil k/2\rceil-1} \sum_{m=k-i}^{\lfloor 2k/3\rfloor-1} \varphi^{i-k-\frac{1}{2}m} \\
&\lesssim \sum_{i=\lfloor k/3\rfloor+1}^{\lceil k/2\rceil-1} \varphi^{i-k} \frac{\varphi^{-\frac{1}{2}(k-i)}\big(1-\varphi^{-\frac{1}{2}(i-k/3+1)}\big)}{1-\varphi^{-1/2}} \\
&\lesssim \frac{1}{\varphi^{\frac{3}{2}k}} \sum_{i=\lfloor k/3\rfloor+1}^{\lceil k/2\rceil-1} \varphi^{\frac{3}{2}i} \lesssim \frac{1}{\varphi^{\frac{3}{4}k}} \lesssim \frac{1}{F_k^{3/4}}. \qquad (5.5.13)
\end{aligned}$$

With respect to the second summation,

$$\begin{aligned}
\sum_{i=\lceil k/2\rceil}^{\lceil 2k/3\rceil-1} \sum_{m=k-i}^{\lfloor 2k/3\rfloor-1} \frac{\log F_k}{\max\{F_i, F_m\}^{3/2}} &\lesssim \log F_k \sum_{i=\lceil k/2\rceil}^{\lceil 2k/3\rceil-1} \Big(\sum_{m=k-i}^{i} \varphi^{-\frac{3}{2}i} + \sum_{m=i+1}^{\lfloor 2k/3\rfloor-1} \varphi^{-\frac{3}{2}m} \Big) \\
&\lesssim \log F_k \sum_{i=\lceil k/2\rceil}^{\lceil 2k/3\rceil-1} k\varphi^{-\frac{3}{2}i} \lesssim \frac{(\log F_k)^2}{\varphi^{\frac{3}{4}k}} \lesssim \frac{(\log F_k)^2}{F_k^{3/4}}. \\
& \qquad (5.5.14)
\end{aligned}$$

Moreover, we obtain

$$\begin{aligned}
\sum_{i=\lceil k/2\rceil}^{\lceil 2k/3\rceil-1}\sum_{m=k-i}^{\lfloor 2k/3\rfloor-1}\frac{F_{i-1}F_{m-1}}{\max\{F_i,F_m\}^{3/2}F_k} &\lesssim \sum_{i=\lceil k/2\rceil}^{\lceil 2k/3\rceil-1}\sum_{m=k-i}^{\lfloor 2k/3\rfloor-1}\varphi^{i+m-k-\frac{3}{2}\max\{i,m\}}\\
&= \sum_{i=\lceil k/2\rceil}^{\lceil 2k/3\rceil-1}\Big(\sum_{m=k-i}^{i}\varphi^{m-k-\frac{1}{2}i}+\sum_{m=i+1}^{\lfloor 2k/3\rfloor-1}\varphi^{i-k-\frac{1}{2}m}\Big)\\
&\lesssim \sum_{i=\lceil k/2\rceil}^{\lceil 2k/3\rceil-1}\varphi^{\frac{1}{2}i-k}+\sum_{i=\lceil k/2\rceil}^{\lceil 2k/3\rceil-1}\varphi^{\frac{1}{2}i-k}\\
&\lesssim \varphi^{-\frac{2}{3}k}+\varphi^{-\frac{2}{3}k}\lesssim\frac{1}{F_k^{2/3}}. \qquad (5.5.15)
\end{aligned}$$

Since $\frac{(\log F_k)^2}{F_k^{3/4}}$ converges faster to 0 than $F_k^{-2/3}$, we obtain a convergence rate of order $F_k^{-2/3}$ of the right-hand side of (5.5.6). By setting $R = F_{\lceil 2k/3\rceil}$ we obtain a convergence rate of order $F_k^{-2/3}$ for $\mathcal{Q}_R(\mathcal{F}_k)$, which completes the proof.

□

Remark. *Note that choosing R differently does not improve our result. Since Equation (5.3.1) contains the factor $\frac{1}{R}$, we need to choose $F_k^{2/3} \lesssim R$. Choosing R larger than that can only increase the second term in (5.3.1). But for this second term we proved a convergence of order $F_k^{-2/3}$ for R of order $F_k^{2/3}$. Hence we can not improve our result using a larger value of R.*

5.6 Remarks

To provide a better understanding of the criterion $\mathcal{Q}_R(Y_N)$ as defined in Equation (5.3.1), we give the following remarks.

Recall that $\mathcal{Q}_R$ with respect to a point set $Y_N = \{\boldsymbol{x}_j\}_{j=1}^N$ and $R > 0$ is given by

$$\mathcal{Q}_R(Y_N) = \frac{1}{R} + \sum_{\substack{0<|\boldsymbol{n}|<R\\ \boldsymbol{n}\in\mathbb{Z}^2\setminus\mathbf{0}}}\Big(\frac{1}{|\boldsymbol{n}|^{3/2}}+\frac{1}{(1+|n_1|)(1+|n_2|)}\Big)\Big|\frac{1}{N}\sum_{j=1}^{N}e^{2\pi i\boldsymbol{n}\cdot\boldsymbol{x}_j}\Big|,$$

where $\boldsymbol{n} = (n_1, n_2) \in \mathbb{Z}^2$ and $|\boldsymbol{n}| = \max\{|n_1|, |n_2|\}$.

The quantity $\mathcal{Q}_R(Y_N)$ is derived from the Fourier coefficient decay of the indicator function for a set with smooth boundary, see [11] for more details. The main term in this bound is $|\boldsymbol{n}|^{-3/2}$. In the following we illustrate this result by a simple example. We consider the Fourier coefficient decay of the indicator function for a disk with radius t, $C_t = \{\boldsymbol{x} \in \mathbb{R}^2 : x_1^2 + x_2^2 \le t^2\}$, which is a convex set with constant curvature.

The Fourier transform of the disk is given by

$$\hat{I}(\boldsymbol{n}) = \iint_{\mathbb{R}^2} 1_{C_t}(\boldsymbol{x}) e^{-2\pi \mathrm{i} \boldsymbol{x}\cdot\boldsymbol{k}} \,\mathrm{d}\boldsymbol{x}.$$

To analyse the decay property of $\hat{I}(\boldsymbol{n})$, let

$$\begin{cases} x_1 = r\cos\theta, \\ x_2 = r\sin\theta, \end{cases} \quad \text{and} \quad \begin{cases} k_1 = |\boldsymbol{n}|\cos\varphi, \\ k_2 = |\boldsymbol{n}|\sin\varphi, \end{cases}$$

with $\theta \in [-\pi, \pi], \varphi \in [-\pi, \pi]$, $r \in [0, t]$, and $|\boldsymbol{n}| = \sqrt{n_1^2 + n_2^2}$. Then we have

$$\begin{aligned} \hat{I}(\boldsymbol{n}) &= \int_{-\pi}^{\pi}\int_0^t r e^{-2\pi \mathrm{i}(r\cos\theta, r\sin\theta)\cdot(|\boldsymbol{n}|\cos\varphi, |\boldsymbol{n}|\sin\varphi)} \,\mathrm{d}r\,\mathrm{d}\theta \\ &= \int_{-\pi}^{\pi}\int_0^t r e^{-2\pi \mathrm{i} r|\boldsymbol{n}|\cos(\theta-\varphi)} \,\mathrm{d}r\,\mathrm{d}\theta \\ &= \int_{-\pi}^{\pi}\int_0^t r e^{-2\pi \mathrm{i} r|\boldsymbol{n}|\cos\phi} \,\mathrm{d}r\,\mathrm{d}\phi \\ &= \int_{-\pi}^{\pi} \frac{(2\pi\mathrm{i}|\boldsymbol{n}|\cos\phi t + 1)e^{-2\pi \mathrm{i} t|\boldsymbol{n}|\cos\phi t} - 1}{4\pi^2|\boldsymbol{n}|^2\cos^2\phi} \,\mathrm{d}\phi. \end{aligned}$$

We have

$$\begin{aligned} &\frac{\mathrm{d}\hat{I}(\boldsymbol{n})}{\mathrm{d}t} \\ =\ & \int_{-\pi}^{\pi} \frac{2\pi\mathrm{i}|\boldsymbol{k}|\cos\phi e^{-2\pi \mathrm{i} t|\boldsymbol{n}|\cos\phi t} + (2\pi\mathrm{i}|\boldsymbol{n}|\cos\phi t + 1)(-2\pi\mathrm{i}|\boldsymbol{n}|\cos\phi)e^{-2\pi \mathrm{i} t|\boldsymbol{n}|\cos\phi t}}{4\pi^2|\boldsymbol{n}|^2\cos^2\phi} \,\mathrm{d}\phi \\ =\ & \int_{-\pi}^{\pi} t e^{-2\pi \mathrm{i} t|\boldsymbol{n}|\cos\phi t} \,\mathrm{d}\phi \\ =\ & 2\pi t\, J_0(2\pi|\boldsymbol{n}|t) \lesssim J_0(|\boldsymbol{n}|), \end{aligned}$$

where J_0 is the Bessel function of the first kind. By the identity

$$\frac{\mathrm{d}}{\mathrm{d}|\boldsymbol{n}|}(|\boldsymbol{n}|J_1(|\boldsymbol{n}|)) = |\boldsymbol{n}|J_0(|\boldsymbol{n}|),$$

we have

$$\hat{I}(\boldsymbol{n}) \lesssim \frac{J_1(|\boldsymbol{n}|)}{|\boldsymbol{n}|}.$$

Since the Bessel function decays proportionally to $1/|\boldsymbol{n}|^{1/2}$, $\hat{I}(\boldsymbol{n})$ thus decays proportionally to $1/|\boldsymbol{n}|^{3/2}$.

To generalize the criterion to higher dimension, we need to know the corresponding Fourier coefficient decay of the indicator function along the intersections of rectangles with certain convex sets. Suppose we have an explicit formula for $\mathcal{Q}_R(Y_N)$ in s dimensions. Then a similar idea to the component-by-component construction discussed in Section 2.1 for lattice rules may be used for constructing good lattice rules by minimizing the criterion $\mathcal{Q}_R$. A good sample set $Y_N = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N-1}\}$ in $[0,1]^s$ can be generated by the following procedure:

- Set $z_1 = 1$.
- For $k = 2, \ldots, s$, assume that we found $z_2, \ldots z_{k-1} \in \{1, \ldots, N-1\}$. Then we search for z_k by minimizing the criterion $\mathcal{Q}_R(Y_N(z_1, \ldots, z_{k-1}, z))$ as a function of z, where

  $$Y_N(z_1, \ldots, z_{k-1}, z) = \big\{\{n(z_1, \ldots, z_{k-1}, z)/N\}, n = 0, 1, \ldots, N-1\big\}$$

  is the rank-1 lattice rule with the generating vector $(z_1, \ldots, z_{k-1}, z)$.

However, the form of $\mathcal{Q}_R$ in higher dimensions is not clear at the moment. We leave the study of the component-by-component construction using $\mathcal{Q}_R$ as a criterion for a good lattice point set for future work.

Chapter 6

Conclusion and outlook

In this thesis we studied the problem of constructing good point sets according to non-uniform distributions by employing the acceptance-rejection samplers. We proved discrepancy bounds for samples generated by the acceptance-rejection sampler using different driver sequences, such as digital nets, stratified inputs and lattice point sets. Explicit constructions of driver sequences which yield a convergence order beyond $N^{-1/2}$ for star-discrepancy in dimension one are proposed.

This topic can be further explored from both theoretical and practical aspects. One may further pursue the construction and implementation of low-discrepancy point sets with respect to non-uniform distributions in high dimension. Not many results are available on this topic. As we discussed in Chapter 5, in [3], Aistleitner and Dick proved an existence result of a low-discrepancy point set whose star-discrepancy is of order $(\log N)^{(3s+1)/2}/N$ for non-uniform measures defined in s-dimension. We proposed explicit constructions of driver sequences which can be used in acceptance-rejection samplers yielding a star-discrepancy of samples according to certain non-uniform densities which converges with order $N^{-2/3}$ in dimension one. A criterion for measuring the goodness of driver sequences has also been introduced. However, the generalization of the criterion to higher dimensions is not available yet. To find a suitable quality criterion is of great interest since then the component-by-component construction of a generating vector of lattice rule can be used to construct good lattice point sets.

In statistical physics and Bayesian statistics it is desirable to compute the mean of a function associated with some partially known probability measure. How to design good quasi-Monte Carlo algorithms for sampling from distributions where the density is not known explicitly, is also interesting to explore. For instance, only the characteristic function of the target distribution may be known. In the scope of Monte Carlo, the acceptance-rejection algorithm can work for sampling from a density function when its characteristic function is of special structure, for example the Polya characteristic function. It is not clear at the moment whether quasi-Monte Carlo methods bring any benefit for this problem.

Additionally, the combination of quasi-Monte Carlo and Markov chain Monte Carlo has the potential for significant improvements in a large number of applications. Some numerical experiments indicate a substantial improvement in the computational cost and accuracy. An essential part of my future research is to develop the theory and the efficient implementation of the MCQMC algorithms, which can be used in various applications in the applied sciences and statistics. For instance, the development and the efficient use of quasi-Monte Carlo methods in applications, like financial mathematics and statistical learning.

Bibliography

[1] C. Aistleitner, J. S. Brauchart and J. Dick, *Point sets on the sphere $\mathbb{S}^2$ with small spherical cap discrepancy*, Discrete Comput. Geom., 48 (2012), pp. 990–1024.

[2] C. Aistleitner and J. Dick, *Functions of bounded variation, signed measures, and a general Koksma-Hlawka inequality*, Acta Arith., 167 (2015), pp. 143–171.

[3] C. Aistleitner and J. Dick, *Low-discrepancy point sets for non-uniform measures*, Acta Arith., 163 (2014), pp. 345–369.

[4] L. Ambrosio, A. Colesanti and E. Villa, *Outer Minkowski content for some classes of closed sets*, Math. Ann., 342 (2008), pp. 727–748.

[5] I. A. Antonov and V. M. Saleev, *An effective method for the computation of λP_τ-sequences*, Zh. Vychisl. Mat. i Mat. Fiz., 19 (1979), pp. 243–245, 271.

[6] F. Barekat and R. Caflisch, *Simulation with Fluctuating and Singular Rates*, Commun Comput Phys., 16 (2014), pp. 287–306.

[7] J. Beck, *On the discrepancy of convex plane sets*, Monatsh. Math., 105 (1988), pp. 91–106.

[8] J. Beck, *Some upper bounds in the theory of irregularities of distribution*, Acta Arith., 43 (1984), pp. 115–130.

[9] C. Botts, W. Hörmann and J. Leydold, *Transformed density rejection with inflection points*, Stat. Comput., 23 (2013), pp. 251–260.

[10] G. E. P. Box and M. E. Müller, *A note on the generation of random normal deviates*, Annals Math. Stat, 29 (1958), pp. 610–611.

[11] L. Brandolini, L. Colzani, G. Gigante and G. Travaglini, *Low-discrepancy sequences for piecewise smooth functions on the two-dimensional torus*, J. Complexity, 33 (2016), pp. 1–13.

[12] L. Brandolini, L. Colzani, G. Gigante and G. Travaglini, *On the Koksma-Hlawka inequality*, J. Complexity, 29 (2013), pp. 158–172.

[13] R. E. Caflisch, *Monte Carlo and quasi-Monte Carlo methods*, Acta Numer., 7 (1998), pp. 1–49.

[14] M. Cambou, M. Hofert and C. Lemieux, *Quasi-random numbers for copula models*, available at arxiv.org/abs/1508.03483 (2016).

[15] S. Chen, *Consistency and convergence rate of Markov chain quasi Monte Carlo with examples*, PhD thesis, Stanford University (2011).

[16] S. Chen, J. Dick and A. Owen, *Consistency of Markov chain quasi-Monte Carlo on continuous state spaces*, Ann. Statist., 39 (2011), pp. 673–701.

[17] N. N. Chentsov, *Pseudorandom numbers for modelling Markov chains*, Comput. Math. Math. Phys., 7 (1967), pp. 218–233.

[18] L. Devroye, *Non-uniform random variate generation*, Springer-Verlag, New York, 1986.

[19] J. Dick and F. Y. Kuo, *Reducing the construction cost of the component-by-component construction of good lattice rules*, Math. Comp., 73 (2004), pp. 1967–1988.

[20] J. Dick, *On the convergence rate of the component-by-component construction of good lattice rules*, J. Complexity, 20 (2004), pp. 493–522.

[21] J. Dick, *Walsh spaces containing smooth functions and quasi-Monte Carlo rules of arbitrary high order*, SIAM J. Numer. Anal., 46 (2008), pp. 1519–1553.

[22] J. Dick, F. Y. Kuo and I. H. Sloan, *High-dimensional integration: the quasi-Monte Carlo way*, Acta Numer., 22 (2013), pp. 133–288.

[23] J. Dick and F. Pillichshammer, *Digital nets and sequences*, Discrepancy theory and quasi-Monte Carlo integration, Cambridge University Press, Cambridge, 2010.

[24] J. Dick and D. Rudolf, *Discrepancy estimates for variance bounding Markov chain quasi-Monte Carlo*, Electron. J. Probab., 19 (2014), pp. 1–24.

[25] J. Dick, D. Rudolf and H. Zhu, *Discrepancy bounds for uniformly ergodic Markov chain quasi-Monte Carlo*, accepted for publication in Ann. Appl. Probab., available at arxiv.org/abs/1303.2423 (2016).

[26] B. Doerr, M. Gnewuch and A. Srivastav, *Bounds and constructions for the star-discrepancy via δ-covers*, J. Complexity, 21 (2005), pp. 691–709.

[27] G. Farin, *Curves and Surfaces for Computer Aided Geometric Design: A Practical Guide (5th Ed.)* Morgan Kaufmann, San Francisco, 2002.

[28] H. Faure, *Discrépance de suites associées à un système de numération (en dimension s)*, Acta Arith., 41 (1982), pp. 337–351.

[29] H. Faure and C. Lemieux, *Improved Halton sequences and discrepancy bounds*, Monte Carlo Methods Appl., 16 (2010), pp. 231–250.

[30] M. Gerber and N. Chopin, *Sequential quasi Monte Carlo*, J. R. Stat. Soc. Ser. B. Stat. Methodol., 77 (2015), pp. 509–579.

[31] P. Glasserman, *Monte Carlo methods in financial engineering*, Springer-Verlag, New York, 2004.

[32] M. Gnewuch, *Bracketing numbers for axis-parallel boxes and applications to geometric discrepancy*, J. Complexity, 24 (2008), pp. 154–172.

[33] J. H. Halton, *On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals*, Numer. Math., 2 (1960), pp. 84–90.

[34] J. M. Hammersley, *Monte Carlo methods for solving multivariable problems*, Ann. New York Acad. Sci., 86 (1960), pp. 844–874.

[35] G. Harman, *Variations on the Koksma-Hlawka inequality*, Unif. Distrib. Theory, 5 (2010), pp. 65–78.

[36] Z. He and A. B. Owen, *Extensible grids: uniform sampling on a space-filling curve*, J. R. Stat. Soc. Ser. B. Stat. Methodol. (2016), pp. 1–15.

[37] S. Heinrich, *The multilevel method of dependent tests*, in Advances in stochastic simulation methods, Stat. Ind. Technol. Birkhäuser Boston, Boston, MA, 2000, pp. 47–61.

[38] S. Heinrich, E. Novak, G. W. Wasilkowski and H. Woźniakowski, *The inverse of the star-discrepancy depends linearly on the dimension*, Acta Arith., 96 (2001), pp. 279–302.

[39] K. Hesse, *A lower bound for the worst-case cubature error on spheres of arbitrary dimension*, Numer. Math., 103 (2006), pp. 413–433.

[40] F. J. Hickernell, *A generalized discrepancy and quadrature error bound*, Math. Comp., 67 (1998), pp. 299–322.

[41] E. Hlawka, *Funktionen von beschränkter Variation in der Theorie der Gleichverteilung*, Ann. Mat. Pura Appl., 54 (1961), pp. 325–333.

[42] W. Hörmann, J. Leydold and G. Derflinger, *Automatic nonuniform random variate generation*, Statistics and Computing, Springer-Verlag, Berlin, 2004.

[43] S. Joe and F. Y. Kuo, *Constructing Sobol′ sequences with better two-dimensional projections*, SIAM J. Sci. Comput., 30 (2008), pp. 2635–2654.

[44] J. F. Koksma, *A general theorem from the theory of uniform distribution modulo 1*, Mathematica, Zutphen. B., 11 (1942), pp. 7–11.

[45] N. M. Korobov, *Approximate evaluation of repeated integrals*, Dokl. Akad. Nauk SSSR, 124 (1959), pp. 1207–1210.

[46] N. M. Korobov, *Teoretiko-chislovye metody v priblizhennom analize*, Gosudarstv. Izdat. Fiz.-Mat. Lit., Moscow, 1963.

[47] P. Kritzer, *Improved upper bounds on the star discrepancy of* (t, m, s)*-nets and* (t, s)*-sequences*, J. Complexity, 22 (2006), pp. 336–347.

[48] L. Kuipers and H. Niederreiter, *Uniform distribution of sequences*, John Wiley & Sons Inc., New York, 1974.

[49] F. Y. Kuo, *Component-by-component constructions achieve the optimal rate of convergence for multivariate integration in weighted Korobov and Sobolev spaces*, J. Complexity, 19 (2003), pp. 301–320.

[50] P. L'Ecuyer, C. Lecot and B. Tuffin, *A Randomized Quasi-Monte Carlo Simulation Method for Markov Chains*, Oper. Res., 56 (2008), pp. 958–975.

[51] P. L'Ecuyer, C. Lécot and B. Tuffin, *Randomized quasi-Monte Carlo simulation of Markov chains with an ordered state space*, in Monte Carlo and quasi-Monte Carlo methods 2004, Springer, Berlin, 2006, pp. 331–342.

[52] P. L'Ecuyer and C. Lemieux, *Recent advances in randomized quasi-Monte Carlo methods*, in Modeling uncertainty: An Examination of Stochastic Theory, Methods, and Applications, Kluwer Academic, Boston, MA, 2002, pp. 419–474.

[53] C. Lemieux, *Monte Carlo and quasi-Monte Carlo sampling*, Springer Series in Statistics, Springer, New York, 2009.

[54] S. P. Meyn and R. L. Tweedie, *Markov chains and stochastic stability*, Communications and Control Engineering Series, Springer-Verlag London, Ltd., London, 1993.

[55] W. J. Morokoff and R. E. Caflisch, *Quasi-Monte Carlo integration*, J. Comput. Phys., 122 (1995), pp. 218–230.

[56] B. Moskowitz and R. E. Caflisch, *Smoothness and dimension reduction in quasi-Monte Carlo methods*, Math. Comput. Modelling, 23 (1996), pp. 37–54.

[57] N. Nguyen and G. Ökten, *The acceptance-rejection method for low-discrepancy sequences*, Monte Carlo Methods Appl., 22 (2016), pp. 133–148.

[58] H. Niederreiter, *Dyadic fractions with small partial quotients*, Monatsh. Math., 101 (1986), pp. 309–315.

[59] H. Niederreiter, *Low-discrepancy and low-dispersion sequences*, J. Number Theory, 30 (1988), pp. 51–70.

[60] H. Niederreiter, *Random number generation and quasi-Monte Carlo methods*, CBMS-NSF Regional Conference Series in Applied Mathematics 63, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1992.

[61] H. Niederreiter and J. M. Wills, *Diskrepanz und Distanz von Maßen bezüglich konvexer und Jordanscher Mengen*, Math. Z., 144 (1975), pp. 125–134.

[62] E. Novak and H. Woźniakowski, *Tractability of multivariate problems. Volume II: Standard information for functionals*, EMS Tracts in Mathematics 12, European Mathematical Society (EMS), Zürich, 2010.

[63] D. Nuyens and R. Cools, *Fast component-by-component construction of rank-1 lattice rules with a non-prime number of points*, J. Complexity, 22 (2006), pp. 4–28.

[64] G. Ökten and A. Göncü, *Generating low-discrepancy sequences from the normal distribution: Box-Muller or inverse transform?*, Math. Comput. Modelling, 53 (2011), pp. 1268–1281.

[65] A. B. Owen, *Monte Carlo theory, methods and examples*, Stanford University, available at statweb.stanford.edu/~owen/mc/ (last accessed at March 2016), 2013.

[66] A. B. Owen, *Monte Carlo variance of scrambled net quadrature*, SIAM J. Numer. Anal., 34 (1997), pp. 1884–1910.

[67] A. B. Owen, *Randomly permuted* (t, m, s)*-nets and* (t, s)*-sequences*, Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing, Lecture Notes in Statistics, 106 (1995), pp. 299–317.

[68] A. B. Owen, *Scrambled net variance for integrals of smooth functions*, Ann. Statist., 25 (1997), pp. 1541–1562.

[69] A. B. Owen, *Scrambling Sobol′ and Niederreiter-Xing points*, J. Complexity, 14 (1998), pp. 466–489.

[70] C. P. Robert and G. Casella, *Monte Carlo Statistical Methods*, Springer-Verlag, New York, 2005.

[71] G. O. Roberts and J. S. Rosenthal, *Variance bounding Markov chains*, Ann. Appl. Probab., 18 (2008), pp. 1201–1214.

[72] M. Rosenblatt, *Remarks on a multivariate transformation*, Ann. Math. Statistics, 23 (1952), pp. 470–472.

[73] W. M. Schmidt, *Irregularities of distribution IX. Collection of articles in memory of Juriĭ Vladimirovič Linnik*, Acta Arith., 27 (1975), pp. 385–396.

[74] W. M. Schmidt, *Lectures on irregularities of distribution*, Tata Institute of Fundamental Research Lectures on Mathematics and Physics 56, Tata Institute of Fundamental Research, Bombay, 1977.

[75] I. H. Sloan and S. Joe, *Lattice methods for multiple integration*, Oxford University Press, New York, 1994.

[76] I. H. Sloan and A. V. Reztsov, *Component-by-component construction of good lattice rules*, Math. Comp., 71 (2002), pp. 263–273.

[77] I. M. Sobol′, *Distribution of points in a cube and approximate evaluation of integrals*, Ž. Vyčisl. Mat. i Mat. Fiz., 7 (1967), pp. 784–802.

[78] W. Stute, *Convergence rates for the isotrope discrepancy*, Ann. Probability, 5 (1977), pp. 707–723.

[79] S. D. Tribble, *Markov chain Monte Carlo algorithms using completely uniformly distribution driving sequences*, PhD thesis, Stanford University (2007).

[80] S. D. Tribble and A. B. Owen, *Construction of weakly CUD sequences for MCMC sampling*, Electron. J. Stat., 2 (2008), pp. 634–660.

[81] J. van der Corput, *Verteilungsfunktionen. I. Mitt.* Proc. Akad. Wet. Amsterdam, 38 (1935), pp. 813–821.

[82] X. Wang and F. J. Hickernell, *Randomized Halton sequences*, Math. Comput. Modelling, 32 (2000), pp. 887–899.

[83] X. Wang, *Improving the rejection sampling method in quasi-Monte Carlo methods*, J. Comput. Appl. Math., 114 (2000), pp. 231–246.

[84] X. Wang, *Quasi-Monte Carlo integration of characteristic functions and the rejection sampling method*, Comput. Phys. Commun., 123 (1999), pp. 16–26.

[85] T. T. Warnock, *Computational investigations of low-discrepancy point sets*, in Applications of number theory to numerical analysis, Academic Press, New York, 1972, pp. 319–343.

[86] A. D. Wyner, *Capabilities of bounded discrepancy decoding*, Bell Systems Tech. J., 44 (1965), pp. 1061–1122.

[87] R.-X. Yue and F. J. Hickernell, *Integration and approximation based on scramble sampling in arbitrary dimensions*, J. Complexity, 17 (2001), pp. 881–897.

[88] R.-X. Yue and F. J. Hickernell, *Strong tractability of integration using scrambled Niederreiter points*, Math. Comp., 74 (2005), pp. 1871–1893.

[89] S. C. Zaremba, *La discrépance isotrope et l'intégration numérique*, Ann. Mat. Pura Appl. (4), 87 (1970), pp. 125–135.

[90] S. K. Zaremba, *Computing the isotropic discrepancy of point sets in two dimensions*, Discrete Math., 11 (1975), pp. 79–92.

[91] H. Zhu and J. Dick, *A discrepancy bound for deterministic acceptance-rejection samplers beyond $N^{-1/2}$ in dimension 1*, Stat. Comput., doi:10.1007/s11222-016-9661-2 (2016).

[92] H. Zhu and J. Dick, *Discrepancy bounds for deterministic acceptance-rejection samplers*, Electron. J. Stat., 8 (2014), pp. 678–707.

[93] H. Zhu and J. Dick, *Discrepancy estimates for acceptance-rejection samplers using stratified inputs*, Proceedings of the MCQMC 2014 conference, Belgium, R. Cools and D. Nuyens (Eds.), Springer (2016), pp. 599–619.