Workshop on

Uniform Distribution and Quasi-Monte Carlo Methods

October 14-18, 2013

as part of the

Radon Special Semester 2013 on

Applications of Algebra and Number Theory

ÖAW Austrian Academy of Sciences

RICAM JOHANN · RADON · INSTITUTE FOR COMPUTATIONAL AND APPLIED MATHEMATICS

"*Metric number theory, lacunary series and systems of dilated functions*"

Christoph Aistleitner Kobe University, Japan

Abstract

By a classical result of Weyl, for any increasing sequence $(n_k)_{k\geq 1}$ of integers the sequence of fractional parts $(\{n_k x\})_{k\geq 1}$ is uniformly distributed modulo 1 for almost all $x \in [0,1]$. Except for a few special cases, e.g. when $n_k = k$, the exceptional set cannot be described explicitly. The exact asymptotic order of the discrepancy of $(\{n_k x\})_{k\geq 1}$ for almost all x is only known in a few special cases, for example when $(n_k)_{k\geq 1}$ is a Hadamard lacunary sequence, that is when $n_{k+1}/n_k \geq q > 1$. In this case of quickly increasing $(n_k)_{k\geq 1}$ the system $(\{n_k x\})_{k\geq 1}$ (or, more generally, $(f(n_k x))_{k\geq 1}$ for a 1-periodic function f) shows many asymptotic properties which are typical for the behavior of systems of *independent* random variables. Precise results depend on a fascinating interplay between analytic, probabilistic and number-theoretic phenomena.

Without any growth conditions on $(n_k)_{k\geq 1}$ the situation becomes much more complicated, and the system $(f(n_k x))_{k\geq 1}$ will typically fail to satisfy probabilistic limit theorems. An important problem which remains is to study the almost everywhere convergence of series $\sum_{k=1}^{\infty} c_k f(kx)$, which is closely related to finding upper bounds for maximal L^2-norms of the form

$$\int_0^1 \left(\max_{1\leq M\leq N} \left| \sum_{k=1}^{M} c_k f(kx) \right| \right)^2 dx.$$

The most striking example of this connection is the equivalence of the Carleson convergence theorem and the Carleson–Hunt inequality for the maximal partial sum of a Fourier series. For general functions f this is a very difficult problem, which is related to finding upper bounds for certain sums involving greatest common divisors.

"*Strong uniformity*"

Jozsef Beck Rutgers University, USA

Abstract

We attempt to develop a new chapter of the theory of Uniform Distribution; we call it Strong Uniformity. In a nutshell it means to combine Lebesgue measure with the classical theory (initiated by H. Weyl in 1916). Our main result is to prove the continuous version of an old conjecture of Khinchin in arbitrary dimension at least two: it is about the strong uniformity of a typical torus line modulo one (or billiard trajectory in a box) starting from the origin. Here Strong means that we test uniformity with an arbitrary measurable set. In the 2-dimensional case we even have Superuniformity, indicating strikingly small polylogarithmic error. Replacing the torus line in a square with a 2-dimensional ray in a 3-cube, we have Super-Duper uniformity, which basically means no error.

"*Discrepancy theory and harmonic analysis*"

Dmitriy Bilyk University of Minnesota, USA

Abstract

Many results in the theory of irregularities of distribution relied on ideas and techniques coming from harmonic analysis. We shall give a brief non-technical overview of applications of Fourier analysis in discrepancy theory, touching upon a number of classical topics in uniform distribution and corresponding analytic methods: discrepancy of sequences (exponential sums), discrepancy with respect to rotated rectangles/balls (Fourier transform/series), discrepancy with respect to axis-parallel rectangles (Haar, Walsh and other orthogonal expansions).

In the second part, we shall discuss discrepancy with respect to rectangles rotated in partial sets of directions, which is an intermediate situation between the aforementioned two cases (all rotations and no rotations). We obtain upper discrepancy bounds using lattices rotated by a carefully chosen angle. The proof strategies reveal connections to Diophantine approximations, Fourier analysis and combinatorics. (This is joint work with X. Ma, J. Pipher, C. Spencer.)

“*Constructing QMC-designs on the sphere – separation and covering properties*”

Johann Brauchart UNSW Sydney, Australia

Abstract

We discuss explicit constructions of configurations on the sphere that are good candidates for QMC-designs. These include spherical digital nets and sequences and spherical lattices derived from their flat counterparts by means of an area preserving map to the sphere.

“*A Belgian view on lattice rules*”

Ronald Cools KU Leuven, Belgium

Abstract

Nowadays the quasi-Monte Carlo community is well aware of the existence of lattice rules and their versatility. There was a time that most texts started with saying that lattice rules are for integrating periodic functions. Many people still think that their number of points must be fixed in advance and that for every other number another rule is needed. These “problems” are more “misunderstandings” and probably delayed the use of lattice rules in practice.

Nowadays lattice rules are studied as just a set of low discrepancy points and it is clear that lattice rules can also be treated as sequences. One could even state that lattice rules are probably the most elegant type of quasi-Monte Carlo point sets: easy to understand, easy to implement and easy to use. (Not everybody agrees with this but as the title suggests, this is a biased view.)

In this talk I will introduce lattice rules from my favorite perspective and I will survey some classical results in this area.

“*Applications of geometric discrepancy*”

Josef Dick UNSW Sydney, Australia

Abstract

Geometric discrepancy measures the uniformity of distribution of a point set. Classical results study the discrepancy of the empirical distribution of a point set from the uniform distribution with respect to boxes. In this talk we consider discrepancy with respect to other test sets. We motivate such measures of uniformity from generating uniformly distributed points on the sphere and from Markov chain Monte Carlo algorithms.

“*Subsequences of automatic sequences and uniform distribution*”

Michael Drmota TU Vienna, Austria

Abstract

Automatic sequences and their number theoretic properties have been intensively studied during the last 20 or 30 years. Since automatic sequences are quite regular (they just have linear subword complexity) they cannot be used as quasi-random sequences. However, the situation changes drastically when one uses proper subsequences, for example the subsequence along primes or squares. It is conjectured that the resulting sequences are normal sequences which could be recently proved (together with C. Mauduit and J. Rivat) for the Thue-Morse sequence along the subsequence of squares. In this way we obtain a new kind of quasi-random sequence.

This kind of research is very challenging and was mainly motivated by the Gelfond problems for the sum-of-digits function. In particular during the last few years there was a spectacular progress due to the Fourier analytic method by C. Mauduit and J. Rivat.

The purpose of this talk is survey some recent developments, in particular on subsequences along $\lfloor n^c \rfloor$ (for some $c > 1$), on polynomial subsequences and on the subsequence of primes. We also present some new result and formulate several conjectures.

"*Atanassov's methods for low-discrepancy sequences*"
Henri Faure Institut de Mathematiques de Luminy, France

Abstract

The aim of this talk is to give an updated overview on upper bounds for low-discrepancy sequences obtained via Atanassov's methods for Halton sequences. We will focus on extensions of these methods in three directions: first generalizations of Halton sequences by means of matrices, then discrepancy upper bounds for (t, s)-sequences and finally discrepancy upper bounds for so-called $(t, \mathbf{e}, s)$-sequences and generalized Niederreiter sequences.

This is joint work with Christiane Lemieux.

"*Optimal randomized algorithms for integration on function spaces with underlying ANOVA decomposition*"
Michael Gnewuch TU Kaiserslautern, Germany

Abstract

In this talk we present upper and lower error bounds for the infinite-dimensional numerical integration problem on weighted Hilbert spaces with norms induced by an underlying ANOVA decomposition. Here the weights model the relative importance of different groups of variables. We have results for randomized algorithms in two different cost models and our error bounds are in both settings sharp in the case of product weights and finite-intersection weights. The constructive upper error bounds are based on randomized multilevel altorithms in the first cost model and randomized changing dimension algorithms in the second cost model.

As example spaces of integrands we discuss Sobolev spaces with different degrees of smoothness. In this setting we use quasi-Monte Carlo multilevel and changing dimension algorithms based on (interlaced) scrambled polynomial lattice rules. These algorithm can obtain higher order convergence rates that are arbitrarily close to the optimal convergence rate.

The talk is based on joint work with Jan Baldeaux (UTS, Sydney) and with Josef Dick (UNSW, Sydney). Our findings are presented in full detail in the following two references:

- J. Baldeaux, M. Gnewuch. Optimal randomized multilevel algorithms for infinite-dimensional integration on function spaces with ANOVA-type decomposition. arXiv:1209.0882v1 [math.NA], Preprint 2012. (http://arxiv.org/abs/1209.0882)
- J. Dick, M. Gnewuch. Optimal randomized changing dimension algorithms for infinite-dimensional integration on function spaces with ANOVA-type decomposition, arXiv:1306.2821v1 [math.NA], Preprint 2013. (http://arxiv.org/abs/1306.2821)

"*Point sets of minimal energy*"
Peter Grabner Graz University of Technology, Austria

Abstract

For a given compact manifold $M \subset \mathbb{R}^{d+1}$ and a set of N distinct points $X_N = \{x_1, \ldots, x_N\} \subset M$, the Riesz s-energy is defined as $E_s(X_N) = \sum_{i \neq j} \|x_i - x_j\|^{-s}$. A configuration X_N^*, which minimises E_s amongst all N-point configurations, is called a minimal energy configuration. The motivation for studying such configurations comes from Chemistry and Physics, where self-organisation of mutually repelling particles under inverse power laws occur. For fixed s and $N \to \infty$ the distribution $\frac{1}{N} \sum_{j=1}^{N} \delta_{x_j^*}$ approaches a continuous limiting measure, which can be described by classical potential theory, if $s < \dim(M)$, and which is normalised Hausdorff measure, if $s \geq \dim(M)$ by a recent result of D. P. Hardin and E. B. Saff.

We collect recent results on the discrepancy of minimal energy point sets on manifolds, especially the sphere.

"*The hybrid spectral test*"
Peter Hellekalek University of Salzburg, Austria

Abstract

The starting point of this paper is the interplay between the construction principle of a sequence and the characters of the compact abelian group that underlies the construction. In case of the Halton sequence in base $\mathbf{b} = (b_1, \ldots, b_s)$ in the s-dimensional unit cube $[0,1)^s$, which is an important type of a digital sequence, this kind of duality principle leads to the so-called **b**-adic function system and provides the basis for the **b**-adic method, which we present in connection with hybrid sequences. This method employs structural properties of the compact group of **b**-adic integers as well as **b**-adic arithmetic to derive tools for the analysis of the uniform distribution of sequences in $[0,1)^s$. We first clarify the point which function systems are needed to analyze digital sequences. Then, we present the hybrid spectral test in terms of trigonometric-, Walsh-, and **b**-adic functions. Various notions of diaphony as well as many figures of merit for rank-1 quadrature rules in Quasi-Monte Carlo integration and for certain linear types of pseudo-random number generators are included in this measure of uniform distribution. Further, discrepancy may be approximated arbitrarily close by suitable versions of the spectral test.

"*Adapting quasi-Monte Carlo methods to simulation problems in weighted Korobov spaces*"
Christian Irrgeher JKU Linz, Austria

Abstract

The computation of expected values of functions depending on Brownian motions occurs in many applications. For example, in finance the valuation of financial derivatives can quite often be reduced to such a problem. A possible way to tackle this problem numerically is to use simulation techniques like quasi-Monte Carlo methods (QMC).

To place special emphasis on the construction method used for the discrete Brownian path makes sense for quasi-Monte Carlo simulation, because it can have a big influence on the efficiency of QMC. Every Brownian path construction method, e.g., Brownian bridge construction or principal component analysis construction, can be represented by an orthogonal transform. Thus, one can use orthogonal transforms to adapt QMC to the underlying problem.

In this talk we will discuss the effect of orthogonal transforms on QMC. Therefore, we set up a Korobov-type space of functions on $\mathbb{R}^d$ based on Hermite polynomials to perform an error analysis and give tractability results.

The talk is based on joint work with Gunther Leobacher.

"*Higher order QMC Galerkin discretization for parametric operator equations*"
Frances Y. Kuo UNSW Sydney, Australia

Abstract

We construct quasi-Monte Carlo methods to approximate the expected values of linear functionals of Galerkin discretizations of parametric operator equations which depend on a possibly infinite sequence of parameters. Such problems arise in the numerical solution of differential and integral equations with random field inputs. We analyze the regularity of the solutions with respect to the parameters in terms of the rate of decay of the fluctuations of the input field. If $p \in (0,1]$ denotes the "summability exponent" corresponding to the fluctuations in affine-parametric families of operators, then we prove that deterministic "interlaced polynomial lattice rules" of order $\alpha = \lfloor 1/p \rfloor + 1$ in s dimensions with N points can be constructed using a fast component-by-component algorithm, in $\mathcal{O}(\alpha\, s\, N \log N + \alpha^2\, s^2 N)$ operations, to achieve a convergence rate of $\mathcal{O}(N^{-1/p})$, with the implied constant independent of s. This dimension-independent convergence rate is superior to the rate $\mathcal{O}(N^{-1/p+1/2})$, for $2/3 \leq p \leq 1$ recently established for randomly shifted lattice rules under comparable assumptions. In our analysis we use a non-standard Banach space setting and introduce "smoothness-driven product and order dependent (SPOD)" weights for which we show fast CBC construction.

This is joint work with Josef Dick (UNSW), Quoc T. Le Gia (UNSW), Dirk Nuyens (KU Leuven), and Christoph Schwab (ETH Zurich)

"*Discrepancy estimates for sequences: new results and open problems*"
Gerhard Larcher JKU Linz, Austria

Abstract

In this talk we will report on some recent results of the author on questions in the theory of irregularities of distribution, and we will state some concrete open problems which are connected to these results.

The main topics will be:
Metric results on the discrepancy of Halton-Kronecker sequences, lower bounds for the discrepancy of digital nets and sequences, and the best possible general lower bound for the discrepancy of sequences in the unit-interval.

"*Software tools for constructing lattice rules*"
Pierre L'Ecuyer Université de Montréal, Canada

Abstract

Lattice rules are a popular classes of quasi-Monte Carlo (QMC) methods for numerical integration. They are very simple to implement and provide a faster convergence rate than standard Monte Carlo (MC) as a function of the sample size n. With random shifts, they can also provide unbiased randomized QMC (RQMC) estimators whose variance converges at a faster rate than MC, for certain classes of functions. But the appropriate rules depend on the class of functions considered. Tables of parameters have been proposed in various places, but based on predefined figures of merit (or discrepancies) that are not necessarily adapted to the application at hand. Moreover, such tables can hardly cover all possible cases of numbers of points or dimension that one may need.

In this talk, we present Lattice Builder, a software tool designed to search for good lattice parameters based on a wide variety of figures of merit with projection-dependent weights that can be selected by the user and tuned to the model that needs to be simulated. It supports various construction methods, based on exhaustive or partial searches, for an arbitrary dimension and number of points. It can also construct rules that are extensible in the dimension and the number of points. In addition to its flexibility, Lattice Builder is, for many applications, fast enough to be executed on-the-fly, when a lattice rule is needed for a given application. Lattice Builder has a command-line interface, which makes it easy to call from other simulation software, as well as a graphical web interface for a user-friendly direct access.

We will summarize the theory behind its design, survey its main features, illustrate how to use it, and provide examples of applications where we compare the behavior of the worst-case error and the RQMC variance for different figures of merit and different choices of weights.

This is joint work with David Munger.

"*Distribution of Rudin-Shapiro sequences along prime numbers*"
Christian Mauduit Institut de Mathematiques de Luminy, France

Abstract

In a recent joint work with Joel Rivat we gave a method to estimate exponential sums over prime numbers for a class of digital functions. The goal of this talk is to present this method and to show that it applies to the study of the distribution of the Rudin-Shapiro sequence and some of its generalizations along prime numbers.

"*G.l.p., optimal coefficients, rank-1 lattice rules*"

Dirk Nuyens KU Leuven, Belgium

Abstract

Lattice rules for numerical integration were introduced by Korobov in 1959. They were constructed to achieve the optimal rate of convergence for numerical integration of functions expressed by a Fourier series with coefficients decaying according to a hyperbolic cross. We call this a Korobov space. Korobov also showed that his "optimal coefficients" in a specific space can form a low-discrepancy sequence in a very simple way. This can be compared to the more recently studied lattice sequences, in a given base b, which make use of an additional bijection on the integers specified by the (integer) radical inverse function (in base b). To control the exponential dependency on the number of dimensions, Sloan and Woźniakowski introduced weighted function spaces in 1998.

The talk will survey the fast component-by-component construction of rank-1 lattice rules in weighted Korobov space. Recently also functions expressed in cosine series were studied by Dick, Nuyens and Pillichshammer (2013) for which the same results as for the Korobov space. The principles behind this cosine space will also be discussed.

In addition to integration it also makes sense to study collocation using these point sets. Spectral collocation and reconstruction methods using Fourier expansions in Korobov space have been studied before in combination with lattice points. In a current manuscript, together with Suryanarayana and Cools, we investigate the use of rank-1 lattice points for the approximation and collocation of d-variate non-periodic functions with frequency support on a hyperbolic cross of cosine series. We show that rank-1 lattice points can be used as collocation points in the approximation of non-periodic functions and these lattice points can be constructed by a component-by-component algorithm.

"*QMC designs on the sphere*"

Ian H. Sloan UNSW Sydney, Australia

Abstract

QMC designs are sequences (X_N) of N-point sets on the unit sphere $S^d \subset R^{d+1}$, which if used for equal weight (or Quasi Monte Carlo, or QMC) numerical integration, give optimal order of convergence as $N \to \infty$, namely $O(N^{-s/d})$, for functions in a Sobolev space $H^s(S^d)$ on the d-dimensional unit sphere. Here $s > d/2$ is the smoothness parameter of the Sobolev space.

Spherical t-designs with a suitably small number of points are prime examples of QMC designs. (A spherical t-design is a finite subset $X_N \subset S^d$ with the characterizing property that a QMC integration rule with nodes X_N integrates exactly all spherical polynomials of degree $\leq t$.) But there are also many other QMC designs: for example, we show that sequences of point sets on S^2 that maximize the sum of the pairwise Euclidean distances form a sequence of QMC designs for $H^{3/2}(S^2)$.

Numerical experiments suggest that many other other familiar sequences of point sets on the sphere (equal area points, spiral points, minimal energy [Coulomb or logarithmic] point sets, and Fekete points) are QMC designs for appropriate ranges of s values.

The talk is based on joint work with Johann Brauchart, Josef Dick, Edward Saff, Robert Womersley and Yu Guang Wang.

"*Generalized van der Corput sequences and permutations of finite fields* $\mathbb{F}_p$"

Alev Topuzoğlu Sabancı University Istanbul, Turkey

Abstract

This is joint work with Florian Pausinger.
Generalized van der Corput sequences in base b are one-dimensional, infinite sequences of real numbers in the interval $[0, 1)$, and are generated by using permutations of the set $\{0, 1, \ldots, b-1\}$.
Faure has shown that particular choices of permutations can improve their uniform distribution properties considerably. Accordingly we define *weak and good families of permutations.* Faure, and Chaix and Faure have shown that such families exist. We give further examples of good and weak families in prime bases by using properties of permutation polynomials of finite fields $\mathbb{F}_p$.

"*Uniformly distributed sequences of partitions*"

Aljoša Volčič University of Calabria, Italy

Abstract

Kakutani introduced in 1976 his "splitting procedure" of $I = [0, 1]$: take any $\alpha \in]0, 1[$ and divide I in two intervals of length α and $1 - \alpha$, respectively. Now take the longest interval of this partition (denoted by $\alpha\omega$, ω is the trivial partition of I) and divide it proportionally to α and $1 - \alpha$. Iterate this procedure to get the sequence $\kappa_n = \alpha^n\omega$. Sooner or later the partition κ_n will have more than one interval of maximal length. This is, for instance, immediately the case if $\alpha = 1/2$. When more than one interval have maximal length, split all of them proportionally to α and $1 - \alpha$. Kakutani proved that such a sequence of partitions is "uniformly distributed".

This beautiful result remained isolated and essentially unnoticed until around 2010, when it has been generalized in the following way: let ρ be any finite (and not trivial) partition of I. Split its longest interval(s) homothetically to ρ and iterate the procedure. This method provides a whole bunch of uniformly distributed sequences of partitions called ρ-refinements, denoted by $\{\rho^n\omega\}$.

The partitions are, as such, not very practical for applications. For instance the binary partitions are u.d, but one has to use at each step 2^n endpoints of the subintervals. If for the computations this number is not sufficient, one has to double the number of points. Of course in this case the emergency exit is clearly indicated by classical results: order the additional points in the van der Corput order and you can efficiently use $2^n + k$ points for any $0 \leq k \leq 2^n$ which suites your need.

For general ρ-refinements there is no such simple way of reordering the endpoints of $\rho^n\omega$, but very satisfactory orderings have been found for special classes of ρ-refinements called LS-sequences. For these sequences (of partitions and of corresponding points) we also have an thorough analysis of the discrepancy.

An interesting byproduct of our studies is the discovery of unexpected connections between a cutting-stacking method which provides an ergodic transformation T whose itaration $\{T^n(0)\}$ coincides with the β-adic van der Corput sequence for $\beta = \Phi$ (the golden ratio) which in turn happens to run through the points produced by Kakutani's splitting procedure corresponding to $\alpha = \Phi^{-1}$.

Thirty years after their introduction, we also have estimates for the discrepancy of the Kakutani sequences of partitions.

"*Tractability of multivariate analytic problems*"

Henryk Wózniakowski Columbia University, USA, and University of Warsaw, Poland

Abstract

Tractability of multivariate problems usually studies problems with finite smoothness. Then we want to know which d-variate problems can be approximated to within ε by using, say, polynomialy many in d and ε^{-1} function values or arbitrary linear functionals.

There is recently a new stream of work for multivariate analytic problems for which we want to answer the usual tractability questions with ε^{-1} replaced by $1 + \log \varepsilon^{-1}$. So far multivariate integration and approximation have been studied over Korobov spaces with exponentially fast decaying Fourier coefficients. This is work of J. Dick, P. Kritzer, G. Larcher, F. Pillichshammer, and the author. There is a natural need to generalize the analysis for more general analytic problems defined over more general spaces.

The goal of this paper is to survey the existing results, present new results, and propose further questions for the study of tractability of multivariate analytic questions.