04401 Abstracts Collection Algorithms and Complexity for Continuous Problems

— Dagstuhl Seminar —

Thomas Müller-Gronbach¹, Erich Novak², Knut Petras³ and Joseph F. Traub⁴

¹ Universität Magdeburg, Germany gronbach@mail.math.uni-magdeburg.de ² Universität Jena, Germany novak@mathematik.uni-jena.de ³ TU Braunschweig, Germany k.petras@tu-bs.de ⁴ Columbia University, USA traub@cs.columbia.edu

Abstract. From 26.09.04 to 01.10.04, the Dagstuhl Seminar 04401 "Algorithms and Complexity for Continuous Problems" was held in the International Conference and Research Center (IBFI), Schloss Dagstuhl. During the seminar, several participants presented their current research, and ongoing work and open problems were discussed. Abstracts of the presentations given during the seminar as well as abstracts of seminar results and ideas are put together in this paper. The first section describes the seminar topics and goals in general. Links to extended abstracts or full papers are provided, if available.

Keywords. Complexity and regularization of ill-posed problems, non-linear approximation, tractability of high-dimensional numerical problems, quasi-Monte Carlo methods, quantum computing, stochastic computation and quantization, global optimization, differential and integral equations

04401 Summary – Algorithms and Complexity for Continuous Problems

T. Müller-Gronbach, E. Novak, K. Petras and J. F. Traub

The goal of this workshop was to bring together researchers from different communities working on computational aspects of continuous problems.

Continuous computational problems arise in many areas of science and engineering. Examples include path and multivariate integration, function approximation, optimization, as well as differential, integral, and operator equations.

Understanding the complexity of such problems and constructing efficient algorithms is both important and challenging.

The workshop was of a very interdisciplinary nature with invitees from, e.g., computer science, numerical analysis, discrete, applied, and pure mathematics, physics, statistics, and scientific computation. Many of the lectures were presented by Ph.D. students.

Compared to earlier meetings, several very active research areas received more emphasis. These include quantum computing, complexity and tractability of high-dimensional problems, stochastic computation, and quantization, which was an entirely new field for this workshop.

Due to strong connections between the topics treated at this workshop many of the participants initiated new cooperations and research projects.

Full Paper: http://drops.dagstuhl.de/opus/volltexte/2005/153

Lower Bounds for Sturm-Liouville and Phase Estimation

Arvid Bessen (Columbia University)

The phase estimation problem is, given a unitary matrix Q and an eigenvector of Q, to approximate the phase of the corresponding eigenvalue. In this paper we obtain a query lower bound for quantum algorithms solving this problem.

Our analysis generalizes existing lower bound approaches to the case where Q is given by controlled powers Q^p of Q, as it is for example in Shor's order finding algorithm.

In the most general setting where we are given controlled arbitrary powers Q^{p_1}, Q^{p_2}, \ldots of Q, we will prove a $\log(1/\varepsilon)$ lower bound for the number of power queries. This bound is tight as shown by a matching upper bound. The bound is derived through a variation of the polynomial approach which uses trigonometric polynomials and a frequency analysis argument.

Upper Bounds on Complexity of Optimization on the Wiener Space with Noise

Jim Calvin (NJIT - Newark)

In this talk we consider the problem of approximating the global minimum of a Wiener process using only sequentially selected observations of the function value corrupted by independent Gaussian noise with mean zero and variance σ^2 . We show that with equispaced nodes the error (in L_2 sense) after n observations satisfies

$$\frac{n^{1/4}}{\sigma^{1/2}}e_n(N_n^u) \to \gamma \,,$$

where γ is a number between 1/2 and 3/2. A slightly better limit can be obtained by choosing the nodes as a regular sequence generated by a beta distribution.

Given any $\delta > 0$ we describe an adaptive algorithm with the property that

$$e_n(N_n^a) = \mathcal{O}\left(n^{-1/2}\log(n)^{1+\delta}\right).$$

For any algorithm, $e_n(N_n) = \mathcal{O}(n^{-1/2})$, and so the adaptive algorithm is optimal up to the logarithmic factor.

Keywords: Global optimization, Wiener process

Fast Component-By-Component Construction of Rank-1 Lattice Rules for (Non-)Primes (Part I)

Ronald Cools (University of Leuven)

Part I: (this part of the talk by Ronald Cools) We restate our previous result which showed that it is possible to construct the generating vector of a rank-1 lattice rule in a fast way, i.e. $O(sn\log(n))$, with s the number of dimensions and n the number of points assumed to be prime. Here we explicitly use basic facts from algebra to exploit the structure of a matrix – which introduces the crucial cost in the construction – to get a matrix-vector multiplication in time $O(n\log(n))$ instead of $O(n^2)$. We again stress the fact that the algorithm works for any tensor product reproducing kernel Hilbert space.

Part II: (this part of the talk by Dirk Nuyens) In the second part we generalize the tricks used for primes to non-primes, by basically falling back to algebraic group theory. In this way it can be shown that also for a non-prime number of points, this crucial matrix-vector multiplication can be done in time $O(n \log(n))$. We conclude that the construction of rank-1 lattice rules in an arbitrary r.k.h.s. for an arbitrary amount of points can be done in a fast way of $O(sn \log(n))$.

Keywords: Numerical integration, cubature/quadrature, rank-1 lattice, component-by-component construction, fast algorithm

Joint work of: Cools, Ronald; Nuyens, Dirk

Optimal Approximation of Elliptic Problems II: Wavelet Methods

Stephan Dahlke (Universität Marburg)

This talk is concerned with optimal approximations of the solutions of elliptic boundary value problems. After briefly recalling the fundamental concepts of optimality, we shall especially discuss best n-term approximation schemes based on wavelets. We shall mainly be concerned with the Poisson equation in Lipschitz domains. It turns out that wavelet schemes are suboptimal in general, but nevertheless they are superior to the usual uniform approximation methods.

Moreover, for specific domains, i.e., for polygonal domains, wavelet methods are in fact optimal. These results are based on regularity estimates of the exact solution in a specific scale of Besov spaces.

Keywords: Elliptic operator equations, worst case error, best n-term approximation, wavelets, Besov regularity

Joint work of: Dahlke, Stephan; Novak, Erich; Sickel, Winfried

Extended Abstract: http://drops.dagstuhl.de/opus/volltexte/2005/138

The Asymptotic Coding Complexity of Stochastic Processes

Steffen Dereich (TU Berlin)

In this talk we consider the quantization and entropy coding problem for Gaussian originals on Banach spaces. We start with stating asymptotic estimates. Next, we present recent results of a detailed analysis of a random strategy in quantization (joint work with M.A. Lifshits).

It turns out that the quality obtained with the random strategy is equal to the inverse of a random small ball function of the underlying measure. We finish the talk with giving the analogues to the above results in the case where the underlying space is even a Hilbert space.

Keywords: Quantization, high resolution coding, small ball function, Gaussian measure

Cyclic Nets for Multivariate Integration

Josef Dick (Univ. of New South Wales)

In this talk we introduce a construction algorithm for cyclic nets, which were recently introduced by Niederreiter. Cyclic nets are a special class of digital nets. Here we exploit the fact that for a given number of points b^m and other given parameters, the number of cyclic nets is b^m .

By using the root mean square worst-case error of randomly digitally shifted point sets for integration in a weighted Sobolev space as selection criteria in our algorithm we are able to show that for any choice of parameters there exists a cyclic net satisfying an upper bound which shows on the one hand that we can achieve the best possible rate of convergence and on the other hand satisfies a tractability error bound.

A similar approach was previously used for polynomial lattice rules by Dick et. al.. The approach here is more general in that we allow digital nets constructed over finite fields of prime power order $q = p^r$, whereas previously this has only been shown for polynomial lattice rules over finite fields of prime order.

We also generalize the construction of cyclic nets, allowing us to also introduce a component-by-component type algorithm. This new construction goes by the name of hyperplane nets.

Though the order of operations of this type of algorithm is increased, we can on the other hand improve the upper bound on the root mean square worst-case error. In this case we can obtain strong tractability (similar upper bounds have previously been shown for lattice rules and polynomial lattice rules constructed by a component-by-component algorithm).

Joint work of: Dick, Josef; Pillichshammer, Friedrich; Pirsic, Gottlieb

Monte Carlo Solution for the Poisson Equation on the Base of Spherical Processes with Shifted Centres

Nina Golyandina (St. Petersburg University)

We consider a class of spherical processes rapidly converging to the boundary (so called Decentred Random Walks on Spheres or spherical processes with shifted centres) in comparison with the standard walk on spheres. The aim is to compare costs of the corresponding Monte Carlo estimates for the Poisson equation. Generally, these costs depend on the cost of simulation of one trajectory and on the variance of the estimate.

It can be proved that for the Laplace equation the limit variance of the estimation does not depend on the kind of spherical processes. Thus we have very effective estimator based on the decentred random walk on spheres. As for the Poisson equation, it can be shown that the variance is bounded by a constant independent of the kind of spherical processes (in standard form or with shifted centres). We use simulation for a simple model example to investigate variance behavior in more details.

Keywords: Poisson equation, Laplace operator, Monte Carlo solution, spherical process, random walk on spheres, rate of convergence

Full Paper: http://drops.dagstuhl.de/opus/volltexte/2005/139

Quantization of Self-Similar Probabilities

Siegfried Graf (Universität Passau)

The asymptotic behaviour of the quantization errors for self-similar probabilities is determined.

Keywords: Quantization, self-similar probabilities

Joint work of: Graf, Siegfried; Luschgy, Harald

Extended Abstract: http://drops.dagstuhl.de/opus/volltexte/2005/140

Numerical Approximation of Parabolic Stochastic Partial Differential Equations

Erika Hausenblas (Universität Salzburg)

The topic of the talk was the time approximation of quasi linear stochastic partial differential equations of parabolic type. The framework was in the setting of stochastic evolution equations.

An error bounds for the implicit Euler scheme was given and the stability of the scheme were considered.

Keywords: Stochastic partial differential equations, stochastic evolution equations, numerical approximation, implicit Euler scheme

Extended Abstract: http://drops.dagstuhl.de/opus/volltexte/2005/141

On the Randomized and Quantum Query Complexity of Elliptic PDE

Stefan Heinrich (TU Kaiserslautern)

The information/query complexity of solving general elliptic partial differential equations in smooth domains is studied in the randomized and quantum setting. Using integral representations via Green's functions matching (up to logarithms) upper and lower bounds are obtained.

Covering Numbers, Vapnik-Cervonenkis Classes and Bounds for the Star-Discrepancy

Aicke Hinrichs (Universität Jena)

The star-discrepancy of a set is one of the main tools to estimate the worst case error of multivariate integration for certain classes of functions. There are rather accurate bounds on the best possible star-discrepancy of an n-point set in the d-dimensional unit cube $[0,1]^d$ for fixed dimension d asymptotically in n. For some applications the dimension d may be so large that it becomes impossible to use enough points such that these bounds give reasonable error estimates.

The question how the discrepancy depends on the dimension d then turns out to be a critical issue.

Recently, S. Heinrich, E. Novak, G. W. Wasilkowski and H. Woźniakowski proved an upper bound on the star discrepancy that shows that it depends only polynomially on d/n. They also showed a lower bound which is rather far from the upper bound as it depends exponentially on d/n. It is the purpose of this talk to discuss how the lower bound can be improved to a polynomial behavior

in d/n. This provides the currently best lower bounds on the star discrepancy for n not excessively large compared with d. The method uses different notions of the size of a set such as covering numbers and Vapnik-Cervonenkis dimension and adapts to a rather general framework.

Upper Error Bounds for Approximations of Stochastic Differential Equations with Markovian Switching

Norbert Hofmann (Universität Frankfurt)

In this talk we consider stochastic differential equations with Markovian switching (SDEwMS). An SDEwMS is a stochastic differential equation with drift and diffusion coefficients depending not only on the current state of the solution but also on the current state of a right-continuous Markov chain taking values in a finite state space.

Consequently, an SDEwMS can be viewed as the result of a finite number of different scenarios switching from one to the other according to the movement of the Markov chain. The generator of the Markov chain is given by transition probabilities involving a parameter which controls the intensity of switching from one state to another. We construct numerical schemes for the approximation of SDE'swMS and present upper error bounds for these schemes. Our numerical schemes are based on a time discretization with constant step-size and on the values of a discrete Markov chain at the discretization points. It turns out that for the Euler scheme a similar upper bound as in the case of stochastic ordinary differential equations can be obtained, while for the Milstein scheme there is a strong connection between the power of the step-size appearing in the upper bound and the intensity of the switching.

Keywords: Stochastic differential equations with Markovian switching, Markov chains, numerical methods, Euler scheme, Milstein scheme

Extended Abstract: http://drops.dagstuhl.de/opus/volltexte/2005/142

Some Complexity Results in d-Variate Global Optimization

Matthias U. Horn (Universität Jena)

We consider a family of function classes which allow functions with several minima and which demand only Lipschitz continuity for smoothness.

We present an algorithm almost optimal for each of these classes.

Keywords: Global optimization, Lipschitz functions, optimal rate of convergence, complexity

Full Paper: http://drops.dagstuhl.de/opus/volltexte/2005/143

Fast Quantum Algorithm For Numerical Gradient Estimation

Stephen Jordan (MIT - Cambridge)

Given a blackbox for f, a smooth real scalar function of d real variables, one wants to estimate the gradient of f at a given point with n bits of precision. On a classical computer this requires a minimum of d+1 blackbox queries, whereas on a quantum computer it requires only one query regardless of d. The number of bits of precision to which f must be evaluated matches the classical requirement in the limit of large n.

Keywords: Quantum, gradient, numerical algorithm

Randomly Shifted Lattice Rules with Unbounded Integrands

Frances Kuo (Univ. of New South Wales)

In recent years there have been many studies of the multivariate integration problem where the integral of a function over the d-dimensional unit cube is approximated by quadrature rules of the equal weight form, with random (Monte Carlo) or deterministically chosen (quasi-Monte Carlo) quadrature points. The integrands in these studies are often assumed to be at least continuous and somewhat smooth. Under the appropriate function space setting, it is known that good randomly shifted lattice rules can be constructed to achieve almost a 1/n rate of convergence independently of the dimension.

However, problems arising from applications are often formulated over \mathbf{R}^d and the typical way of transforming such integral into the unit cube using the inverse cumulative normal distribution almost inevitably leads to an integrand which is unbounded near the boundary of the cube.

We define a space of functions which are unbounded over the unit cube. The function space is a weighted tensor-product reproducing-kernel Hilbert space. We carry out the worst-case analysis in this space and show that good randomly shifted lattice rules can be constructed to achieve a worst-case error smaller than the Monte Carlo error. This in a way provides a theoretical justification of the robustness of quasi-Monte Carlo rules as observed in practice - QMC often perform no worse than MC even for very difficult integrands!

Keywords: Multivariate integration, randomly shifted lattice rules, worst-case error

Joint work of: Kuo, Frances; Sloan, Ian; Waterhouse, Ben

Complexity of Multivariate Feynman-Kac Path Integration

Marek Kwas (Columbia University)

We consider the multivariate Feynman-Kac path integration problem in the worst-case, randomized and quantum settings for a general class of d initial value and potential functions. For smooth d-variate functions, it has been proved in (*) that the worst case complexity suffers from the curse of dimensionality in d. We show that in both the randomized and quantum settings the curse of dimensionality is broken, i.e., the number of function evaluations and/or quantum queries required to compute an ε -approximation has a bound independent on d and depends polynomially on $1/\varepsilon$.

The exponents of these polynomials are at most 2 in the randomized setting and at most 1 in the quantum setting. Hence we have an exponential speedup over the worst case setting and the quadratic speedup of the quantum setting over the randomized setting.

(*) M. Kwas, Y. Li: Worst case complexity of multivariate Feynman-Kac path integration. J. Complexity, 19, 730–743 (2003)

Keywords: Feynman-Kac formula, path integration, information-based complexity, quantum algorithms

Functional Quantization and Entropy for Stochastic Processes

Harald Luschgy (Universität Trier)

Let X be a Gaussian process and let U denote the Strassen ball of X. A precise link between the L^2 -quantization error of X and the Kolmogorov (metric) entropy of U in a Hilbert space setting is established. In particular, the sharp asymptotics of the Kolmogorov entropy problem is derived. The condition imposed is regular variation of the eigenvalues of the covariance operator. Good computable quantizers for Gaussian and diffusion processes and their numerical efficieny are discussed.

Keywords: Functional quantization, entropy, product quantizers

Joint work of: Luschgy, Harald; Pagès, Gilles

Full Paper: http://drops.dagstuhl.de/opus/volltexte/2005/144

Optimal Non-Linear Approximation Using Sets of Finite Pseudo-Dimension

Vitali Maiorov (Technion - Haifa)

We consider optimal non-linear approximations of multivariate functions by manifolds of finite pseudo-dimension. For example, the spaces of univariate spline-functions with n free knots or rational function of degree n are manifolds of pseudo-dimension of order n. In this paper we adduce some examples of manifolds in the multivariate case. We obtain asymptotic estimates for the pseudo-dimensional n-widths of Sobolev's classes $W_p^{r,d}$ in the space L_q in the case of non-compact embedding, that is, when r/d=1/p-1/q. Note that in the case the well-known n-widths, including the Kolmogorov and entropy n-widths, do not converge to zero.

Keywords: Pseudo-dimension, n-widths, Sobolev's classes

Stratified Sampling for Risk Management

Peter Mathé (Weierstraß Institut - Berlin)

We discuss the approximation of Value at Risk (VaR) and other quantities relevant to risk management. One of the core problems in this context is the approximation of the distribution of quadratic forms of Gaussian vectors. It appears as an intermediate problem in the variance reduction techniques proposed by Glasserman et. al. as well as in so-called Δ - Γ -normal approaches.

The purpose is to show that sampling methods are faster than Fourier inversion for a range of practical problems.

The theoretical results are supported by a case study based on real-life problems, showing that sampling methods are faster than Fourier inversion for all but the smallest problems. Thus the use of randomized methods is recommended and the issue of variance reduction becomes important.

Stratification methods – especially randomized orthogonal arrays – turn out to lead to the most effective methods in terms of accuracy per computational cost.

Keywords: Risk management, randomized orthogonal arrays

Joint work of: Mathé, Peter; Jaschke, Stefan

On the Complexity of Computing Multi-Homogeneous Bézout Numbers

Klaus Meer (Univ. of Southern Denmark - Odense)

We study the question how difficult it is to compute the multi-homogeneous Bézout number for a polynomial system of given number n of variables and given support A of monomials with non-zero coefficients.

We show that this number is NP-hard to compute. It cannot even be efficiently approximated within an arbitrary, fixed factor unless P = NP.

Keywords: Multi-homogeneous Bézout numbers, number of roots of polynomials, approximation algorithms

Joint work of: Meer, Klaus; Malajovich, Gregorio

 $\textit{Full Paper:} \quad \text{http://drops.dagstuhl.de/opus/volltexte/} \\ 2005/146$

On the Representation of Smooth Functions on the Sphere Using Finitely Many Bits

Hrushikesh N. Mhaskar (California State Univ. - Los Angeles)

We discuss the construction of a parsimonious representation of smooth functions on the Euclidean sphere using finitely many bits, in the sense of metric entropy. The smoothness of the functions is measured by Besov (approximation) spaces. The bit representation is obtained by uniform quantization on the values of a polynomial frame operator at scattered sites on the sphere.

For each cap, one can identify a certain number of bits, commensurable with the local smoothness of the target function on that cap and the volume of that cap, and obtained using the values of the frame operator near that cap. The polynomial frame operator is calculated using either spherical harmonic coefficients or, in the case of uniform approximation, values of the function at scattered sites on the sphere. The localization properties of the polynomial frame operator are demonstrated by a characterization of local smoothness of the target function near a point in terms of the values of these operators near the point in question.

Keywords: Metric entropy, polynomial frames, approximation on the sphere

Approximation of Stochastic Delay Differential Equations

Thomas Müller-Gronbach (Universität Magdeburg)

We introduce a new scheme for pathwise approximation of scalar stochastic delay differential equations with constant time lag. Our algorithm is based on equidistant evaluation of the driving Brownian motion and is simply obtained by replacing iterated Ito-integrals by products of appropriate Brownian increments in the definition of the Milstein scheme. The piecewise linear interpolation of the new scheme is asymptotically optimal with respect to the mean square L_2 -error within the class of all pathwise approximations that use observations of the driving Brownian motion at equidistant points. Moreover, for a large class of equations our scheme is also asymptotically optimal for mean square approximation of the solution at the final time point. Our asymptotic optimality results are complemented by a comparison with the Euler scheme based on exact error formulas for a linear test equation. This comparison demonstrates the superiority of the new method even for a very small number of discretization points.

Joint work of: Müller-Gronbach, Thomas; Hofmann, Norbert

Stochastic Differential Equations with Additive Fractional Noise: Numerical Schemes and Error Bounds

Andreas Neuenkirch (TU Darmstadt)

Stochastic differential equations driven by a fractional Brownian motion with Hurst parameter H>1/2, can be understood - under standard smoothness assumptions on the drift resp. diffusion coefficient - as pathwise Riemann-Stieltjes integral equations.

In this talk, we will consider the case of additive noise and study pathwise approximations of these SDEs with respect to a L^2 mean square error criterion. We will derive upper and lower error bounds and also consider the question of optimal approximation schemes.

Keywords: Fractional brownian motion, stochastic differential equations, Euler scheme, upper and lower error bounds

Optimal Approximation of Elliptic Problems by Linear and Nonlinear Mappings

Erich Novak (Universität Jena)

We study the optimal approximation of the solution of an operator equation Au = f by linear mappings of rank n and compare this with the best n-term approximation with respect to an optimal Riesz basis. We consider worst case errors, where f is an element of the unit ball of a Hilbert space.

We apply our results to boundary value problems for elliptic PDEs on an arbitrary bounded Lipschitz domain. Here we prove that approximation by linear mappings is as good as the best n-term approximation with respect to an optimal Riesz basis. Our results are concerned with approximation, not with computation.

Our goal is to understand better the possibilities of nonlinear approximation.

Keywords: Elliptic operator equation, worst case error, linear approximation method, nonlinear approximation method, best n-term approximation, Bernstein widths, manifold widths

Joint work of: Novak, Erich; Dahlke, Stephan; Sickel, Winfried Full Paper: http://drops.dagstuhl.de/opus/volltexte/2005/147

Fast Component-By-Component Construction of Rank-1 Lattice Rules for (Non-)Primes (Part II)

Dirk Nuyens (University of Leuven)

Part I: (this part of the talk by Ronald Cools) We restate our previous result which showed that it is possible to construct the generating vector of a rank-1 lattice rule in a fast way, i.e. $O(sn\log(n))$, with s the number of dimensions and n the number of points assumed to be prime. Here we explicitly use basic facts from algebra to exploit the structure of a matrix – which introduces the crucial cost in the construction – to get a matrix-vector multiplication in time $O(n\log(n))$ instead of $O(n^2)$. We again stress the fact that the algorithm works for any tensor product reproducing kernel Hilbert space.

Part II: (this part of the talk by Dirk Nuyens) In the second part we generalize the tricks used for primes to non-primes, by basically falling back to algebraic group theory. In this way it can be shown that also for a non-prime number of points, this crucial matrix-vector multiplication can be done in time $O(n \log(n))$. We conclude that the construction of rank-1 lattice rules in an arbitrary r.k.h.s. for an arbitrary amount of points can be done in a fast way of $O(sn \log(n))$.

Keywords: Numerical integration, cubature/quadrature, rank-1 lattice, component-by-component construction, fast algorithm

Joint work of: Nuyens, Dirk; Cools, Ronald

Full Paper: http://drops.dagstuhl.de/opus/volltexte/2005/148

Fast Eigenvector Approximation for Phase Estimation

Anargyros Papageorgiou (Columbia University)

We present a quantum algorithm preparing an initial state for phase estimation. The algorithm produces a good approximation of the necessary eigenvector at low cost. The algorithm can be used in the approximation of low-order eigenvalues of continuous eigenvalue problems, such as the Sturm-Liouville eigenvalue problem. The classical complexity (deterministic and randomized) of approximating the ground state eigenvalue of the Sturm-Liouville problem is polynomial in $1/\varepsilon$, where ε is the desired accuracy. We use the initial state preparation algorithm in the study of the quantum complexity of this problem with power queries.

We show tight bounds for the qubit complexity and the query complexity.

Keywords: Quantum algorithms, phase estimation, complexity

Joint work of: Papageorgiou, Anargyros; Jaksch, Peter; Woźniakowski, Henryk

Numerical Differentiation from Viewpoint of Regularization Theory

Sergei V. Pereverzev (Johann Radon Forschungsinstitut - Linz)

Numerical differentiation is a classical example of ill-posed problem, and a number of techniques have been developed for it. Any of them should take into account that even small perturbations of the function to be differentiated may lead to large errors in the computed derivative.

Therefore, it is natural to assume that information about differentiated function is noisy. As a result, traditional methods for numerical differentiation have to be combined with regularization. These methods fall into two categories: methods using non-discretized noisy data and methods based on discrete noisy information. They yield satisfactory results when the smoothness of the function to be differentiated is given precisely. However, in many applications it is not the case, and it was a surprise for us that almost all papers on numerical differentiation do not address this issue. In the talk we are going to discuss a new approach to the regularization of the methods belonging to both of above-mentioned categories.

Using recent results of regularization theory we propose stable and orderoptimal methods for numerical differentiation which do not use any information concerning the smoothness of the function to be differentiated.

Keywords: Numerical differentiation, regularization, adaptation

Joint work of: Pereverzev, Sergei V.; Shuai, Lu

On the Complexity of Linear Parabolic Problems

Knut Petras (Braunschweig)

We consider linear parabolic initial value problems of second order in several dimensions.

The initial condition is supposed to be fixed and we investigate the computational complexity if the coefficients of the parabolic equations may vary in certain function spaces. Using the parametrix method (or Neumann series), we prove that lower bounds for the error of numerical methods are related to lower bounds for integration problems. On the other hand, approximating the Neumann series with Smolyak's method, we show that the problem is not much harder than a certain approximation problem. For Hölder classes on compact sets, e.g., lower and upper bounds are close together, such that we have an almost optimal method.

Keywords: Partial differential equations, parabolic problems, Smolyak method, optimal methods

Joint work of: Petras, Knut; Ritter, Klaus

Full Paper: http://drops.dagstuhl.de/opus/volltexte/2005/149

Monte Carlo Methods with Few Random Bits for Integration and Integral Equations

Harald Pfeiffer (Universität Jena)

Monte Carlo methods are algorithms that involve randomness. They are widely applied in multivariate integration and integral equations. As source of randomness a method typically uses random numbers from [0,1], and most of the classical methods use about $d\,n$ of those random numbers where d is the dimension and n the number of function values.

Here, we replace random numbers from [0,1] with random bits from $\{0,1\}$ and we want to use only a small number of them. We consider problems for that (deterministic and) general Monte Carlo methods are well studied: the approximate integration of functions from Hölder and Sobolev spaces and the local solution of Fredholm integral equations with smooth data.

We show that these problems are tractable for Monte Carlo methods with random bits. Moreover, we construct methods that have the optimal order of complexity, which is the same as for general Monte Carlo. The methods for integration use only about $d \log n$ random bits, those for integral equations about $d \log^3 n$. In some cases we can indicate how the overall cost of the method depends on the dimension. Concerning, for example, integral equations with continuously differentiable kernels and right-hand sides the optimal cost of deterministic methods with error ε is of order $(1/\varepsilon)^{2d}$. We obtain methods with a cost of $c((1/\varepsilon)^2 + d\log^3(1/\varepsilon))$ or $cd^5(1/\varepsilon)^{2d/(d+1)}$. Our approach to the problems is to reduce them to the approximation of means.

Keywords: Monte Carlo methods, random bits, numerical integration, integral equations

Information-based Nonlinear Approximation: An Average Case Setting

Leszek Plaskota (University of Warsaw)

Nonlinear approximation has usually been studied under deterministic assumption and complete information about the underlying functions.

We assume only partial information and we are interested in the average case error and complexity of approximation. It turns out that the problem can be essentially split into two independent problems related to average case nonlinear (restricted) approximation from complete information, and average case unrestricted approximation from partial information. The results are then applied to average case piecewise polynomial approximation, and to average case approximation of real sequences.

This work was partially done with M. Kon and G.W. Wasilkowski.

Keywords: Average case setting, nonlinear approximation, information-based complexity

Extended Abstract: http://drops.dagstuhl.de/opus/volltexte/2005/150

Is the Suzuki Non-Existence Theorem a Limiting Factor for the Rate of Convergence of Feynman-Kac Path Integrals?

Cristian Predescu (Univ. California - Berkeley)

The standard technique for the evaluation of the density matrix in statistical quantum mechanics is via Lie-Trotter formula. In a slightly more general setting, Suzuki has shown that no Trotter-like formulas converge asymptotically faster than quadratically, with the number of time slices. This negative result has long been considered as setting a limit on the rate of convergence of path integrals. I shall present several mathematical arguments demonstrating that Suzuki's result does not put any limitation on the existence of faster direct path integral methods.

Algorithms having cubic and quartic asymptotic convergence are presented. The problem of designing algorithms having arbitrary convergence orders can be reduced to the resolution of a set of non-linear functional equations involving generalized moments of a standard Brownian motion.

Whether this set of functional equations has solutions or not for orders greater or equal to 5 is an open problem, the resolution of which is of interest to the chemical physicist.

Non-Uniform Time Discretization and Lower Bounds for Stochastic Heat Equations

Klaus Ritter (TU Darmstadt)

We study algorithms for approximation of the mild solution of stochastic heat equations on the spatial domain $]0,1[^d]$. The error of an algorithm is defined in L_2 -sense. We derive lower bounds for the error of every algorithm that uses a total of N evaluations of one-dimensional components of the driving Wiener process W. For equations with additive noise we derive matching upper bounds and we construct asymptotically optimal algorithms. The error bounds depend on N and d, and on the decay of eigenvalues of the covariance of W in the case of nuclear noise. In the latter case the use of non-uniform time discretizations is crucial.

Keywords: Stochastic heat equation, non-uniform time discretization, minimal errors, upper and lower bounds

Joint work of: Ritter, Klaus; Müller-Gronbach, Thomas

Full Paper: http://drops.dagstuhl.de/opus/volltexte/2005/151

Optimal Approximation of Elliptic Problems by Linear and Nonlinear Mappings III

Winfried Sickel (Universität Jena)

We study two types of nonlinear widths for the embedding

$$B_{p,q}^{-s+t}(\Omega) \hookrightarrow B_{2,q}^{-s}(\Omega), \qquad t > d\left(\frac{1}{p} - \frac{1}{2}\right)_*$$

and compare this with the known behavior of the linear widths. It turns out that the nonlinear widths (representing some sort of nonlinear approximation) tend faster to zero (in order) than the linear widths if and only if 0 . Our treatment is based on earlier work of DeVore, Howard, Micchelli, Kyriazis, Leviatan, and Tikhomirov.

Keywords: Nonlinear approximation, nonlinear widths

Joint work of: Sickel, Winfried; Dahlke, Stephan; Novak, Erich

Randomly Shifted Lattice Rules with Unbounded Integrands - Average Case Interpretation

Ian H. Sloan (Univ. of New South Wales)

This talk, which describes joint work with Ben Waterhouse and Frances Kuo, revisits material in an earlier talk in this Seminar by Frances Kuo.

In that talk multiple integrals over the unit cube were seen to arise in a natural way, if a standard mapping is used to transform a multidimensional expected value with Gaussian probability distributions to the unit cube. In the earlier talk the worst-case error was studied for integrands in an appropriate reproducing kernel Hilbert space of unbounded functions. In this talk, in contrast, the function space of unbounded functions on the unit cube is equipped with a probability measure, and the error is studied in an average case setting. The construction is chosen in such a way that the covariance matrix in the average case setting is equal to the reproducing kernel in the worst-case setting. The result obtained in the previous talk then allows us to infer that there exists a good choice of randomly shifted lattice rule which, on the average, has smaller error than the simple Monte Carlo method.

Keywords: Quasi-Monte Carlo method, error, average-case, worst-case, multiple integration, Monte Carlo method

Joint work of: Sloan, Ian H.; Kuo, Frances; Waterhouse, Ben

An Adaptive Algorithm for ODE, PDE and SDE

Anders Szepessy (KTH Stockholm)

A posteriori error estimates suitable for adaptive refinement are well established. I will focus on the fundamental, but less studied, issue of convergence rates of adaptive algorithms: I will describe an adaptive algorithm applied to ordinary, stochastic and partial differential equations with proven convergence rates. The algorithm reduces the maximal error indicator with a given factor in each iteration or stops with the error asymptotically bounded by the tolerance using the optimal mesh (up to problem independent factors).

In particular I will explain:

- how to measure optimal convergence rates for approximation of functionals of the solution.
- why convergence of the error density is always useful and subtle in the case of stochastic and partial differential equations,
- an example of weak approximation of expected values, depending on solutions to Ito differential equations by the Monte Carlo Euler method, in the case of stopped and reflected boundary conditions.

The motivation for adaptive time steps is that stopped boundary conditions with N standard uniform time steps yield $N^{-1/2}$ convergence rate, while the

corresponding rate is N^{-1} without boundary. This talk will show that this double scale problem can be approximated with the optimal N^{-1} convergence rate using N adaptive time steps.

High-Dimensional Integrals Related to Grid Computing (Part II)

Shu Tezuka (IBM - Kanagawa)

In this talk, I present high-dimensional integrals which represent the expected execution time for a job to be completed on a PC grid. The dimension of the integrals is equal to the number of PCs on the grid. I will discuss a class of isotropic integrals obtained by assuming that the utilization of all PCs follow independent identical probability distributions. I will show some numerical results on the comparison between quasi-Monte Carlo and Monte Carlo methods to compute such isotropic integrals.

 $\begin{tabular}{ll} $Keywords:$ & Grid computing, high-dimensional integrals, quasi-Monte Carlo methods \end{tabular}$

Polynomial-Time Algorithms for Multivariate Linear Problems with Finite-Order Weights; Worst Case Setting

Gregorz W. Wasilkowski (University of Kentucky)

We consider approximation of linear multivariate problems defined over weighted tensor product Hilbert spaces with finite-order weights. This means we consider functions of d variables that can be represented as sums of functions of at most q^* variables. Here, q^* is fixed (and presumably small) and d may be arbitrarily large.

For the univariate problem, d=1, we assume we know algorithms $A_{1,\varepsilon}$ that use $O(\varepsilon^{-p})$ function or linear functional evaluations to achieve an error ε in the worst case setting. Based on these algorithms $A_{1,\varepsilon}$, we provide a construction of polynomial-time algorithms $A_{d,\varepsilon}$ for the general d-variate problem with the number of evaluations bounded roughly by $\varepsilon^{-p}d^{q^*}$ to achieve an error ε in the worst case setting.

Keywords: Multivariate integration, multivariate approximation, complexity, polynomial-time algorithms, finite-order weights

Joint work of: Wasilkowski, Gregorz W.; Woźniakowski, Henryk

Full Paper: http://drops.dagstuhl.de/opus/volltexte/2005/152

Scattered Data Approximation

Holger Wendland (Universität Göttingen)

In practice, one often faces the problem of reconstructing a multivariate function from a given, finite data set. In the simplest case, such a data set consists of data values $f_j = f(x_j) \in \mathbf{R}$, $1 \le j \le N$, coming from an unknown function f at certain data sites $X = \{x_1, \ldots, x_N\} \subseteq \Omega \subseteq \mathbf{R}^d$, and interpolation is the most obvious reconstruction method. In general, the data sites are scattered over the region Ω , having no structure at all.

Approximation by positive definite kernels tries to solve this reconstruction problem by fixing a symmetric kernel $\Phi: \Omega \times \Omega \to \mathbf{R}$. Then, the approximant is chosen from the finite space $\{\Phi(.,x_j): x_j \in X\}$. The assumption on Φ being positive definite leads to a well-posed problem.

In this talk I will focus on the following topics:

- error estimates in Sobolev spaces for reconstruction processes from scattered data,
- the construction of a fast reconstruction and evaluation algorithm,
- (if time permits) examples from surface reconstruction in computer-aided design and from fluid-structure-interaction in aeroelasticity.

Keywords: Approximation orders, positive definite functions, radial basis functions, efficient algorithms

Quantum Parametric Integration in Sobolev Spaces

Carsten Wiegand (TU Kaiserslautern)

We study parametric integration from the Sobolev space $W_p^r([0,1]^{d_1+d_2})$ to $L_p([0,1]^{d_1})$. We show upper and lower complexity bounds in the quantum setting using results from discrete parametric integration.

Joint work of: Wiegand, Carsten; Heinrich, Stefan

Multivariate Integration in $C^{\infty}([0,1]^d)$ Is Not Strongly Tractable

Jakub O. Wojtaszczyk (University of Warsaw)

It has long been known that the multivariate integration problem for the unit ball in $C^r([0,1]^d)$ is intractable for fixed finite r. H. Woźniakowski has recently conjectured that this is true even if $r=\infty$. In my talk I will show a proof of a partial result in this direction. I will show that the multivariate integration problem, for infinitely differentiable functions all of whose partial derivatives are bounded by one, is not strongly tractable.

We show that for a given $\varepsilon>0$ and sufficiently large d we can find, given a deterministic algorithm using n function values, a function on the d-dimensional cube with all partial derivatives bounded by one, the integral of which is greater then $1-\varepsilon$ and yet the function assumes the value 0 in all n points checked by the algorithm. This is enough to show that even with the very limiting assumptions multivariate integration is not strongly tractable.

Keywords: Multivariate integration, strong tractability

Thresholding With Respect to Bases

Przemyslaw Wojtaszczyk (University of Warsaw)

Various thresholding procedures are widely used in many numerical algorithms, in image processing, denoising etc. In this talk I will describe approximation properties of coefficient thresholding in various L_p norms. I will consider expansions with respect to trigonometric system, Haar wavelet on d-dimensional space and tensor Haar system on d-dimensional space.

Keywords: Wavelet, thresholding