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Book of Abstracts

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Detecting hidden structure with deep kernel learning

Author and Presenter: Bastian **Bohn** (University of Bonn, Germany)

Co-authors: Michael **Griebel** (University of Bonn, Germany)
Christian **Rieger** (University of Bonn, Germany)

Abstract

In this talk we deal with chained approximations by linear combinations of kernel translates and briefly discuss their relationship to deep neural networks. We introduce a representer theorem for these kinds of approximations for both the finite-data setting and for the case of infinitely many data points. We provide numerical examples to illustrate how function reconstruction and machine learning tasks can be tackled. We also illustrate how these approximation systems are detected and exploit intrinsically low-dimensional structures in a data set.

Data compression using quasi-Monte Carlo

Author and Presenter: Josef **Dick** (University of New South Wales, Australia)

Co-author: Michael **Feischl** (TU Wien, Austria)

Abstract

Large data sets are nowadays ubiquitous in many areas. Fitting suitable models poses unique computational challenges. We discuss a method of compressing data when one wants to fit a model minimizing the two-norm of the residuals. The method uses low-discrepancy point sets as representative points together with weights which depend on the data set.

Sparse-grid polynomial interpolation approximation and integration for parametric and stochastic elliptic PDEs with lognormal inputs

Author and Presenter: Dũng **Dinh** (Vietnam National University, Hanoi, Vietnam)

Abstract

By combining a certain approximation property in the spatial domain, and weighted ℓ_2-summability of the Hermite polynomial expansion coefficients in the parametric domain obtained in [1] and [2], we investigate linear non-adaptive methods of fully discrete polynomial interpolation approximation as well as fully discrete weighted quadrature methods of integration for parametric and stochastic elliptic PDEs with lognormal inputs. We explicitly construct such methods and prove corresponding convergence rates of the approximations by them. The linear non-adaptive methods of fully discrete polynomial interpolation approximation are sparse-grid collocation methods which are certain sums taken over finite nested Smolyak-type indices sets $G(\xi)$ parametrized by $\xi > 0$, of mixed tensor products of dyadic scale successive differences of spatial approximations of particular solvers, and of successive differences of their parametric Lagrange interpolating polynomials. The Smolyak sparse grids in the parametric domain are constructed from the roots of Hermite polynomials or their improved modifications.

Moreover, they generate fully discrete weighted quadrature formulas in a natural way for integration of the solution to parametric and stochastic elliptic PDEs and its linear functionals, and the error of the corresponding integration can be estimated via the error in the Bochner space $L_1(\mathbb{R}^\infty, V, \gamma)$ norm of the generating methods where γ is the Gaussian probability measure on $\mathbb{R}^\infty$ and V is the energy space.

Our analysis leads to auxiliary convergence rates in parameter ξ of these approximations when ξ going to ∞. For a given $n \in \mathbb{N}$, we choose ξ_n so that the cardinality of $G(\xi_n)$ which in some sense characterizes computation complexity, does not exceed n, and hence obtain the convergence rates in increasing n, of the fully discrete polynomial approximation and integration.

References

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[2] M. Bachmayr, A. Cohen, D. Dũng and C. Schwab: *Fully discrete approximation of parametric and stochastic elliptic PDEs*, SIAM J. Numer. Anal., 55:2151-2186, 2017.

Construction of rank-1 lattice rules by a smoothness-independent component-wise digit-by-digit construction

Author and Presenter: Adrian **Ebert** (KU Leuven, Belgium)

Co-authors: Peter **Kritzer** (RICAM, Austria)
Dirk **Nuyens** (KU Leuven, Belgium)
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Abstract

In this talk, we introduce a component-wise digit-by-digit method (CBC-DBD) for the construction of rank-1 lattice rules in spaces of periodic functions with prescribed decay for the Fourier coefficients and associated smoothness $\alpha > 1$. This method is an extension of the construction algorithm established by Korobov in [1] to the weighted function space setting. We show that the introduced CBC-DBD algorithm constructs lattice rules with $N = 2^n$ points which achieve the almost optimal worst-case error convergence rates in the studied function spaces. Due to the usage of a quality function which is independent of the smoothness α, the algorithm constructs lattice rules which achieve these convergence rates uniformly for all smoothness parameters $\alpha > 1$. The involved proof technique is essentially different from common proofs for component-wise construction methods. Furthermore, we derive conditions on the weights under which the mentioned error bounds are independent of the dimension. The CBC-DBD algorithm can be implemented in a fast manner such that the construction only requires $\mathcal{O}(sN \ln N)$ operations, where $N = 2^n$ is the number of lattice points and s denotes the dimension, making it competitive with the common fast CBC algorithm, see, e.g., [2]. This fast construction is easy to implement and does not rely on the use of fast Fourier transformations (FFTs). Numerical results confirm our theoretical findings.

References

[1] N.M. Korobov: *On the computation of optimal coefficients*, Dokl. Akad. Nauk SSSR, 26:590-593, 1982.

[2] 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(1):4-28, 2006.

Simplex stochastic collocation for piecewise smooth functions with kinks

Author and Presenter: Jochen **Garcke** (Universität Bonn, Germany)

Co-author: Barbara **Fuchs** (Fraunhofer SCAI, Germany)

Abstract

We consider the treatment of higher dimensional non-smooth functions with kinks. For example, such kinks can arise in the uncertainty quantification of quantities of interest for gas networks. This is due to the regulation of the gas flow, pressure, or temperature. But, one can exploit that for each sample in the parameter space it is known if a regulator was active or not, which can be obtained from the result of the corresponding numerical solution. This information can be exploited in a stochastic collocation method based on simplices.

We approximate the function separately on each smooth region by polynomial interpolation and obtain an approximation to the kink. Note that one does not need information about the exact location of kinks, but only an indicator assigning each sample point to its smooth region. We obtain a global order of convergence of $(p+1)/d$, where p is the degree of the employed polynomials and d the dimension of the parameter space. We show the empirical performance of the approach in up to four dimensions on synthetic test functions and for the uncertainty quantification of the expected pressure of a node in a gas network caused by uncertain input data.

References

[1] B. Fuchs and J. Garcke: *Simplex stochastic collocation for piecewise smooth functions with kinks*, International Journal for Uncertainty Quantification, 2019, accepted.

Multilevel quasi-Monte Carlo methods for a random elliptic eigenvalue problem

Author and Presenter: Alexander **Gilbert** (Universität Heidelberg, Germany)

Co-author: Robert **Scheichl** (Universität Heidelberg, Germany)

Abstract

Motivated by uncertainty quantification for the neutron diffusion criticality problem, we will study an elliptic eigenvalue problem with coefficients that depend on infinitely many stochastic parameters. The stochasticity in the coefficients causes the eigenvalues and eigenfunctions to also be stochastic, and so our goal is to compute the expectation of the minimal eigenvalue. In practice, to approximate this expectation, one must:

1) truncate the stochastic dimension;

2) discretise the eigenvalue problem in space (e.g., by finite elements); and

3) apply a quadrature rule to estimate the expected value.

In this talk, we will present a multilevel (quasi-)Monte Carlo method for approximating the expectation of the minimal eigenvalue, which is based on a hierarchy of finite element meshes and truncation dimensions. To improve the sampling efficiency over Monte Carlo we will use a randomly shifted lattice rule to generate the sampling points, for which the sampling error can converge at a rate of $1/N$ as compared with the Monte Carlo rate of $1/\sqrt{N}$. Also, to make each eigenproblem solve on a given level more efficient, we utilize the two-grid finite element method for eigenproblems to obtain the eigenvalue on the fine mesh from the coarse eigenvalue (and eigenfunction) with a single linear solve.

A Quasi-Monte Carlo Method for PDE-constrained optimization under uncertainty

Author and Presenter: Philipp **Guth** (University of Mannheim, Germany)

Co-authors: Vesa **Kaarnioja** (UNSW Sydney, Australia)
Frances **Kuo** (UNSW Sydney, Australia)
Claudia **Schillings** (University of Mannheim, Germany)
Ian **Sloan** (UNSW Sydney, Australia)

Abstract

In this work we apply a quasi-Monte Carlo (QMC) method to an optimal control problem constrained by an elliptic partial differential equation (PDE) equipped with an uncertain diffusion coefficient. In particular the optimization problem is to minimize the expected value of a tracking type cost functional with an additional penalty on the control. The uncertain coefficient in the PDE is parametrized by a countably infinite number of terms via a Karhunen-Loève expansion (KLE) and the expected value is considered as an infinite-dimensional integral in the corresponding parameter space.

We discretize the optimization problem by truncating the KLE after s terms, approximating the expected value by an n-point QMC rule in s dimensions and approximating the solution of the PDE using finite elements (FE). It is shown that the discretization error of the solution to the optimization problem is bounded by the discretization error of the adjoint state. For the convergence analysis the latter is decomposed into truncation error, QMC error and FE error, which are then analysed separately. Numerical experiments confirming our theoretical convergence results will be presented.

Algorithms and complexity for stochastic integration in various function classes

Author and Presenter: Stefan **Heinrich** (University of Kaiserslautern, Germany)

Abstract

Inspired by a recent paper of Eisenmann and Kruse [1] we study algorithms for and the complexity of stochastic integration with respect to the Wiener sheet measure $\int_{[0,1]^d} f(t)dW_t$ of stochastic functions f with the following types of regularity: f is assumed to belong to $L_u(\Omega, X)$, where $1 \le u < \infty$ and X is

- a Sobolev space $X = W_p^r([0,1]^d)(r \in \mathbb{N}, 1 \le p \le \infty)$, or
- a Besov space $X = B_{pp}^r([0,1]^d)(r \in \mathbb{R}; 0 < r < \infty, 1 \le p \le \infty)$ (also called Sobolev-Slobodeckij space), or
- a Bessel-potential space $X = H_p^r([0,1]^d)(r \in \mathbb{R}; 0 < r < \infty; 1 < p < \infty)$.

In all cases it is assumed that $r/d > 1/p - 1/2$. Information about f consists of function values while that about W_t may be function values or scalar products with polynomials of a given degree. Both deterministic and randomized algorithms are considered. We determine the order of the complexity, which includes finding and analyzing algorithms of optimal order and proving matching lower bounds. This extends results from [1], where upper bounds for the one-dimensional case $X = B_{pp}^r([0,1])$ with $0 < r < 2$, $2 \le p < \infty$ were established, and from [2], where only deterministic integrands were considered.

References

[1] M. Eisenmann and R. Kruse: *Two quadrature rules for stochastic Itô-integrals with fractional Sobolev regularity*, arXiv:1712.08152.

[2] S. Heinrich: *Complexity of stochastic integration in Sobolev classes*, J. Math. Anal. Appl., 476:177-195, 2019.

Quasi-Monte Carlo integration in uncertainty quantification of elliptic PDEs with log-Gaussian coefficientsy

Author and Presenter: Lukas **Herrmann** (ETH Zurich, Switzerland)

Co-author: Christoph **Schwab** (ETH Zurich, Switzerland)

Abstract

Quasi-Monte Carlo (QMC) rules are suitable to overcome the curse of dimension in the numerical integration of high-dimensional integrands. Also the convergence rate of essentially first order is superior to Monte Carlo sampling. We study a class of integrands that arise as solutions of elliptic PDEs with log-Gaussian coefficients. In particular, we focus on the overall computational cost of the algorithm. We prove that certain multilevel QMC rules have a consistent accuracy and computational cost that is essentially of optimal order in terms of the degrees of freedom of the spatial Finite Element discretization for a range of infinite-dimensional priors.

References

[1] L. Herrmann and Ch. Schwab: *QMC integration for lognormal-parametric, elliptic PDEs: local supports and product weights*, Numer.Math., 141(1):63-102, 2019.

[2] L. Herrmann and Ch. Schwab: *Multilevel quasi-Monte Carlo integration with product weights for elliptic PDEs with lognormal coefficients*, to appear in ESAIM:M2AN.

[3] L. Herrmann: *Strong convergence analysis of iterative solvers for random operator equations*, SAM report, 2017-35, in review.

Higher order QMC rules for uncertainty quantification using periodic random variables

Author and Presenter: Vesa **Kaarnioja** (UNSW Sydney, Australia)

Co-authors: Frances **Kuo** (UNSW Sydney, Australia)
Ian **Sloan** (UNSW Sydney, Australia)

Abstract

A popular model for the parametrization of random fields in uncertainty quantification is given by the so-called affine model, where the input random field is assumed to depend on independent, uniformly distributed random variables in a linear manner. In this talk, we consider a different model for the input random field, where the random variables enter the input field as periodic functions instead. The field can be constructed to have the same mean and covariance function as the affine random field. This setting allows us to construct simple lattice QMC rules that obtain higher order convergence rates, which we apply to elliptic PDEs equipped with random coefficients.

References

[1] V. Kaarnioja, F.Y. Kuo and I.H. Sloan: *Uncertainty quantification using periodic random variables*, Preprint arXiv:1905.07693 [math.NA].

Multiple lattice rules for multivariate L_∞ approximation in the worst-case setting

Author and Presenter: Lutz **Kämmerer** (TU Chemnitz, Germany)

Abstract

Abstract We consider multivariate periodic functions that belong to reproducing kernel Hilbert spaces. A recent work [1] of Cobos, Kühn, and Sickel proved that the worst case approximation error measured in the sup-norm, where one is allowed to use at most n linear information of the function in order to compute the approximation, can be realized by the exact Fourier partial sum that involves the potentially n most important trigonometric monomials. Note that the aforementioned importance only depends on the reproducing kernel Hilbert space, since we consider a worst case approximation error.

We present an approach for approximating this Fourier partial sum by means of a specific sampling strategy that is based on rank-1 lattice sampling and investigate the corresponding worst case sampling error, i.e., the approximation error with respect to the required number of sampling values. It turns out that our sampling strategy requires a number of approximately $9n \ln n$ sampling values in order to approximate the Fourier partial sum such that the worst case sampling error is almost as good as the worst case approximation error of the exact Fourier partial sum - up to some multiplicative factor $3 \ln n + 1$. In particular, this relation of the approximation errors to the corresponding sampling errors does not depend on the dimension and holds even in pre-asymptotic settings. Further applications of the general theoretical result improve known estimates of the worst case sampling error for rank-1 lattices substantially including those that incorporates tractability considerations.

Besides the extremely convincing approximation properties, a further great advantage of the suggested sampling method is that the computation of the approximants can be realized using a highly efficient FFT approach. Thus, we present an excellently suitable sampling strategy even for reasonable possibly pre-asymptotic settings.

References

[1] F. Cobos, T. Kühn and W. Sickel: *Optimal approximation of multivariate periodic Sobolev functions in the sup-norm*, J. Funct. Anal., 270:4196-4212, 2016.

Methods for large-scale and high-dimensional kernel cubature

Author and Presenter: Toni **Karvonen** (Aalto University, Finland)

Co-authors: Chris **Oates** (Newcastle University & Alan Turing Inst., UK)
Simo **Särkkä** (Aalto University, Finland)

Abstract

Kernel cubature rules, worst-case optimal numerical integration methods in reproducing kernel Hilbert spaces, can be interpreted as *probabilistic numerical methods* [1] and used for statistical quantification of uncertainty due to incomplete knowledge of the integrand. Motivated by this equivalence, we develop computational methods for efficient construction of large-scale and potentially high-dimensional kernel cubature rules. For N data points, the naive implementation of kernel cubature rules is based on solving a linear system of N equations. The resulting cubic time and quadratic memory cost in N are serious computational bottlenecks. We show how relatively flexible *fully symmetric sets*, obtained from given vectors via coordinate permutations and sign-changes, can be exploited for efficient computation of the weights of kernel cubature rules for up to millions of points. If the point set is a union of J fully symmetric sets, time complexity is reduced from $\mathcal{O}(N^3)$ to $\mathcal{O}(J^3 + JN)$ and memory complexity from $\mathcal{O}(N^2)$ to $\mathcal{O}(J^2)$. This talk is mainly based on the articles [2, 3], but we also discuss some other recent approaches based on *sparse grids* [4] and a combination of *low discrepancy points and shift-invariant kernels* [5].

References

[1] F.-X. Briol, C. J. Oates, M. Girolami, M. A. Osborne and D. Sejdinovic: *Probabilistic integration: A role in statistical computation?* Statistical Science, 34(1):1-22, 2019.

[2] T. Karvonen and S. Särkkä: *Fully symmetric kernel quadrature*, SIAM Journal on Scientific Computing, 40(2):A697-A720, 2018.

[3] T. Karvonen, S. Särkkä and C. J. Oates: *Symmetry exploits for Bayesian cubature methods*, To appear in Statistics and Computing, 2019.

[4] J. Oettershagen: *Construction of Optimal Cubature Algorithms with Applications to Econometrics and Uncertainty Quantification*, PhD thesis, Institut für Numerische Simulation, Universität Bonn, 2017.

[5] J. Rathinavel and F. Hickernell: *Fast automatic Bayesian cubature using lattice sampling*, Preprint, arXiv:1809.09803v1, 2018.

The kernel tensor-product multi-level method

Author and Presenter: Rüdiger **Kempf** (University Bayreuth, Germany)

Co-author: Holger **Wendland** (University Bayreuth, Germany)

Abstract

In applications such as machine learning and uncertainty quantification, one of the main tasks is to reconstruct an unknown function from given data with data sites lying in a high dimensional domain. This task is usually even for relatively small domain dimensions numerically difficult.

We propose a new reconstruction scheme by combining the well-known kernel multi-level technique in low dimensional domains with the anisotropic Smolyak algorithm, which allows us to derive a high dimensional interpolation scheme. This new method has significantly lower complexity than traditional high dimensional interpolation schemes.

In this talk, I will give an introduction to the topics of kernel multi-level and anisotropic Smolyak algorithms before providing a convergence result for this new Kernel Tensor-Product Multi-Level method. If time permits, I will also give numerical examples.

Tensor numerical modeling of the collective electrostatic potentials of many-particle systems

Author and Presenter: Venera **Khoromskaia** (Max-Planck-Institute, Germany)

Abstract

The novel tensor-structured numerical methods appeared as bridging of the algebraic tensor decompositions and the nonlinear approximation theory on separable low-rank representation of multivariate functions and operators [1, 2]. Nowadays the rank-structured tensor approach facilitates new means for numerical modeling of long-range potentials in many-particle systems. The method of grid-based assembled tensor summation of the electrostatic potentials on $(L \times L \times L)$ 3D finite lattices [4] exhibits the computational complexity of the order of $O(L)$ which is much less than $O(L^3)$ in traditional Ewald-type summation. The canonical tensor rank of the collective potential of a finite 3D rectangular lattice system (containing millions of particles) is proven to be as low as a rank for a single reference tensor for a Newton kernel. For lattices with multiple impurities the tensor rank is increased by a small factor [2].

Recent range-separated (RS) tensor format [3] applies to many-particle systems of general type. These can be the free space electrostatic potentials of large bio-molecules or the multidimensional scattered data modeled by radial basis functions. The main advantage of the RS tensor format is that the rank of the canonical/Tucker tensor representing the sum of long range contributions from all particles in the collective potential depends only logarithmically on the number of particles N. Partitioning of long and short range parts of the potentials is performed simply by sorting vectors of the generating Newton kernel. The interaction energies and forces of the many-particle system are computed by using only the long-range part of the collective potential, with representation complexity $O(n \log N)$, where n is the univariate grid size. The basic tool for calculation of the RS tensor representation is the reduced higher order SVD (RHOSVD) introduced in [5]. The representation complexity of the short range part is $O(N)$ with a small prefactor independent on the number of particles. The numerical examples are presented.

References

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[2] V. Khoromskaia and B.N. Khoromskij: *Tensor Numerical Methods in Quantum Chemistry*, De Gruyter, Berlin, 2018.

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Old and new tensor formats for PDE driven applications in many dimensions

Author and Presenter: Boris N. **Khoromskij** (Max-Planck-Institute, Germany)

Abstract

Rank-structured tensor approximation of functions and operators by using the traditional canonical (CP), Tucker and tensor train (TT) formats allows the numerical calculus with linear complexity scaling in dimension. Further data-compression to the logarithmic scale can be achieved by using the quantized-TT (QTT) approximation. The novel range-separated (RS) tensor format is capable for the efficient low-rank approximation in the numerical modeling of many-particle systems in $\mathbb{R}^d$. We discuss how the tensor numerical methods apply to the solution of complicated multidimensional problems in the PDE driven applications, and for the efficient representation and analysis of large multi-dimensional data. In particular, we describe

- The RS tensor decomposition of the Dirac delta and elliptic operator inverse with application to the Poisson-Boltzmann equation in bio-molecular modeling;
- An example on how the QTT and RS tensor formats apply in machine learning for modeling and analysis of scattered multi-dimensional data;
- How the tensor numerical methods apply in stochastic homogenization of the elliptic PDEs in random media, and in the control problems constrained by PDEs in $\mathbb{R}^d$.

The details can be found in the research monograph [1], and in the recent papers [2-5].

References

[1] B.N. Khoromskij: *Tensor Numerical Methods in Scientific Computing*, De Gruyter Verlag, Berlin, 2018.

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[3] B.N. Khoromskij: *Range-separated tensor representation of the discretized multi-dimensional Dirac delta and elliptic operator inverse*, E-Preprint, arXiv:1812.02684v1, 2018.

[4] V. Khoromskaia, B.N. Khoromskij and F. Otto: *Numerical study in stochastic homogenization for elliptic PDEs: convergence rate in the size of representative volume elements*, E-Preprint, arXiv:1903:12227v1, 2019.

[5] G. Heidel, V. Khoromskaia, B. Khoromskij and V. Schulz: *Tensor approach to optimal control problems with fractional d-dimensional elliptic operator in constraints*, E-Preprint, arXiv:1809.01971v2, 2018.

Adaptive approximation on cones

Author and Presenter: Peter **Kritzer** (Austrian Academy of Sciences, Austria)

Co-authors: Yuhan **Ding** (Misericordia University, USA)
Fred J. **Hickernell** (Illinois Institute of Technology, USA)
Simon **Mak** (Georgia Institute of Technology, USA)

Abstract

In this talk, we discuss adaptive approximation algorithms for general multivariate linear problems where the sets of input functions are non-convex cones. While it is known that adaptive algorithms perform essentially no better than non-adaptive algorithms for convex input sets, the situation may be different for non-convex sets. A typical example considered is function approximation based on series expansions. Given an error tolerance, we use series coefficients of the input to construct an approximate solution such that the error does not exceed this tolerance. We consider the situation where we can bound the norm of the input based on a pilot sample, and the situation where we keep track of the decay rate of the series coefficients of the input. Besides, presenting an error analysis, we also discuss the information cost of our algorithms and the computational complexity of our problems, and we identify conditions under which we can avoid a curse of dimensionality.

Lattice algorithms for multivariate approximation in periodic spaces with general weight parameters

Author and Presenter: Frances Y. **Kuo** (UNSW Sydney, Australia)

Co-authors: Ronald **Cools** (KU Leuven, Belgium)
Dirk **Nuyens** (KU Leuven, Belgium)
Ian H. **Sloan** (UNSW Sydney, Australia)

Abstract

We provide the theoretical foundation for the component-by-component construction of lattice algorithms for multivariate L_2 approximation in the worst case setting, for functions in a periodic space with general weight parameters. Our construction leads to an error bound that achieves the best possible rate of convergence for lattice algorithms. This work is motivated by PDE applications in which bounds on the norm of the functions to be approximated require special forms of weight parameters (so-called POD weights or SPOD weights), as opposed to the simple product weights covered by the existing literature. Our result can be applied to other lattice-based approximation algorithms, including kernel methods or splines.

A spectral method for the stochastic Stokes equations on the sphere

Author and Presenter: Quoc Thong **Le Gia** (UNSW, Australia)

Co-author: Joseph **Peach** (UNSW, Australia)

Abstract

We construct numerical solutions to a stochastic Stokes equation on the unit sphere with additive isotropic noise. The noise is expanded in a Karhunen-Loève expansion in terms of the Hodge decomposition of tangential vector fields on the sphere. The approximation of the noise will give rise to a high dimensional approximation problem. Under certain assumptions on the angular power spectrums of the random noise, a mean square error estimate of the random solution is given. Numerical experiments are carried out to illustrate the theory.

Lattice rules in Chebyshev space

Author and Presenter: Dirk **Nuyens** (KU Leuven, Belgium)

Co-authors: Frances **Kuo** (UNSW Sydney, Australia)
Giovanni **Migliorati** (Sorbonne University, France)
Fabio **Nobile** (EPFL, Switzerland)

Abstract

Lattice rules mainly wander around in "Periodic space", i.e., for continuous and smooth functions defined on the Torus. Here we follow lattice rules on a trip through Chebyshev space. We map from Chebyshev space to cosine space and then further to Fourier space. This enables us to study lattice rules for function approximation in Chebyshev space. Fast DCTs can be used to map point values to frequency representation and visa versa. We provide efficient algorithms for CBC style construction of good lattice rules for approximation.

Exponential ReLU DNN expression of holomorphic maps in high dimension

Author and Presenter: Joost A. A. **Opschoor** (ETH Zürich, Switzerland)

Co-authors: Christoph **Schwab** (ETH Zürich, Switzerland)
Jakob **Zech** (MIT, USA)

Abstract

We consider the approximation of analytic maps $u : [-1,1]^d \to \mathbb{R}$ by deep ReLU neural networks, for a possibly large input dimension $d \in \mathbb{N}$. We assume quantitative control of the domain of holomorphy, i.e. u admits a holomorphic extension to a Bernstein polyellipse $\mathcal{E}_{\rho_1} \times \ldots \times \mathcal{E}_{\rho_d} \subset \mathbb{C}^d$ with semiaxis sums $\rho_i > 1$, containing $[-1,1]^d$. We establish exponential convergence in terms of the neural network size N, as the error in Lipschitz norm $W^{1,\infty}([-1,1]^d)$ is shown to decay as $O(\exp(-bN^{1/(d+1)}))$ for a constant $b > 0$ determined by $\{\rho_j\}_{j=1}^d$. In addition, we discuss deep neural networks with a so-called "rectified power unit" (RePU) activation function, which approximate u with convergence of the order $O(\exp(-cN^{1/d}))$ for $c > 0$ depending on $\{\rho_j\}_{j=1}^d$.

References

[1] J.A.A. Opschoor, Ch. Schwab and J. Zech: *Exponential ReLU DNN expression of holomorphic maps in high dimension.* Technical Report 2019-35, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2019.

A modified fast component-by-component construction of rank-1 lattice points in weighted spaces

Author and Presenter: Onyekachi **Osisiogu** (RICAM, Austria)

Co-authors: Adrian **Ebert** (NUMA, KU Leuven, Belgium)
Peter **Kritzer** (RICAM, Austria)
Dirk **Nuyens** (NUMA, KU Leuven, Belgium)

Abstract

Lattice rules are of high benefit in practice because their implementation can be accomplished by very effective construction algorithms. In this talk, we describe a modified component-by-component method (CBC) for rank-1 lattice rules such that the quality function is independent of the smoothness parameter α and has a connection with the worst-case error. We study this method for the case when N is prime. The CBC constructed lattice rules achieve almost optimal order of convergence (which is independent of the weights) and we show that with suitable weights conditions the error bounds can be made independent of the dimensions. We present fast implementation of the construction (with the help of the techniques introduced by Dirk Nuyens and Ronald Cools [2]) and analyze the computational complexity. We further show numerical experiments to compare the error convergence with the classical CBC construction.

References

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[2] 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(1):4-28, 2006.

Tractability properties of discrepancy

Author and Presenter: Friedrich **Pillichshammer** (Johannes Kepler University, Linz)

Co-author: Josef **Dick** (University of New South Wales, Australia)

Abstract

Discrepancies are quantitative measures for the irregularity of distribution of point sets in $[0;1]^d$ which are closely related to the error of quasi-Monte Carlo (QMC) integration rules. Classical results consider discrepancy with respect to its asymptotic dependence when the size N of a point set tends to infinity. In this sense optimal results are known, but often these results give no information on the pre-asymptotic scale, especially when the dimension d is large.

In 2001 Heinrich, Novak, Wasilkowski and Woźniakowski [1] initiated the study of the dependence of discrepancy on the dimension d with a remarkable result for the star discrepancy. They showed that for every N and d there exists a N-point set in $[0;1]^d$ with classical star discrepancy of at most $C\sqrt{d/N}$, where C is a positive constant independent of N and d. Since then a lot of papers on this topic with exciting results have appeared. Nevertheless, a lot of problems are still open.

In this talk we give a review of this topic and present some new results concerning the periodic L_2 discrepancy and the discrepancy with respect to the exponential Orlicz norm.

References

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A spline dimensional decomposition for high-dimensional uncertainty quantification

Author and Presenter: Sharif **Rahman** (The University of Iowa, USA)

Co-author: Ramin **Jahanbin** (The University of Iowa, USA)

Abstract

A spline dimensional decomposition (SDD) of a square-integrable random variable, comprising hierarchically ordered measure-consistent orthonormal basis splines (B-splines) in independent random variables, is introduced. A dimensionwise decomposition of a spline space into orthogonal subspaces, each spanned by a reduced set of measure-consistent orthonormal B-splines, results in SDD. Using the modulus of smoothness, the SDD approximation is shown to converge in mean-square to the correct limit. Analytical formulae are proposed to calculate the second-moment properties of a truncated SDD approximation for a general output random variable in terms of the expansion coefficients involved. Numerical results from an elastostatic problem in 15 stochastic dimensions indicate that a low-degree SDD approximation with an adequate mesh size generates a significantly more accurate estimate of the output variances than a high-order approximation from existing polynomial chaos expansion or polynomial dimensional decomposition. The SDD method proposed is most suitable in the presence of locally nonlinear or nonsmooth behavior found in applications.

Robust solver in a quantized tensor format for electronic structure calculations

Author and Presenter: Maxim **Rakhuba** (ETH Zurich, Switzerland)

Abstract

The idea of reshaping an array with 2^d elements into a multidimensional $2 \times \cdots \times 2$ array and then applying tensor-train (TT) decomposition is known under the name quantized TT decomposition (QTT).

It has been shown in a number of works that arrays arising in the discretization of certain PDEs allow for QTT representation with a small number of parameters. However, the quest for robust and at the same time efficient QTT algorithm to solve PDEs with three (and more) physical dimensions is not over yet. In this talk, we address this problem using the example of PDEs arising in electronic structure calculations with a new algorithm. The proposed algorithm is capable of solving PDEs discretized using 2^{100} grid points within minutes of computational time on a laptop.

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Efficient reliability analysis by combining uncertain measurement data, Bayesian model updating and reduced order modeling

Author and Presenter: Annika **Robens-Radermacher** (BAM, Germany)

Co-authors: Felix **Held** (BAM, Germany)
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Abstract

One of the main challenges regarding our civil infrastructure is the efficient operation over their complete design lifetime while complying with standards and safety regulations. Thus, costs for maintenance or replacements must be optimized while still ensuring specified safety levels. This requires an accurate estimate of the current state as well as a prognosis for the remaining useful life (RUL). Currently, this is often done by regular manual or visual inspections within constant intervals. However, the critical sections are often not directly accessible or impossible to be instrumented at all. In this case, model-based approaches can be used where a numerical model of the structure is set up. Based on this numerical model, a prognosis of the future performance of the structure, e.g. the failure probability, can be computed. The main challenge in this approach is the calibration and validation of the model based on uncertain measurement data. Therefore, model updating approaches which are inverse optimization processes are applied. This requires a huge number of computations of the same numerical model with slightly different model parameters. In reliability analyses, the failure probability of a structure is estimated. The failure probability is defined as an integral of a n-dimensional density function over the failure domain. Usually, it cannot be computed analytically. It is estimated by evaluating the integral function at a huge number of sample points. Thereby, each sample evaluation includes the computation of the numerical model with again slightly different model parameters. For that reason, model updating as well as reliability analyses become computationally very expensive for real applications.

The aim of this contribution is to increase the efficiency of structural model updating and the subsequent reliability analysis by using the advantages of reduced order models. Model reduction is a popular concept to decrease the computational effort of complex numerical simulations. Coupling a reduced model of the structure of interest with a Bayesian model updating approach or a reliability analysis to estimate the failure probability can reduce the computational cost of such analyses drastically. First, the reduced order model of the investigated mechanical structure (a cross-section of a T-beam bridge) is derived. In this contribution, the Proper Generalized Decomposition (PGD) method [1, 2] is used to bypass the curse of dimensionality. The key idea of this method is to use a separated representation for the unknown coordinates including also model parameters. In this case, a numerical abacus is obtained, providing the structural response for all parameter congurations.

Secondly, the PGD reduced model is used in the Bayesian model updating procedure. Measurement data as well as numerical models suffer from different kinds of errors. For a given prior distribution as well as a likelihood function, samples of the a posterior distribution are drawn using a Metropolis-Hasting

algorithm [3]. At each sample, the deviation between numerical model and measurement is computed by the computationally inexpensive evaluation of the PGD solution function instead of the expensive computation of a full order model.

Third, a reliability analysis with the PGD surrogate model and the identified distributions of the random model parameters is developed. For that purpose, an importance sampling [4] using the subset idea [5] for a proper choice of the importance density is applied. Using such a variance-reducing sampling algorithm reduces the number of sample points in general. By evaluating the computationally inexpensive PGD solution at each sample point instead of a full order model, a computationally efficient reliability analysis is carried out. The influences of using a PGD reduced order model in Bayesian model updating and reliability analyses is discussed by means of a numerical example of a bridge model. The main influences on the accuracy of the solution are the mode truncation and mesh discretization. Furthermore, the convergence of the identication is demonstrated and estimation of the failure probability is provided.

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Parallel cross interpolation for high-precision calculation of high-dimensional integrals

Author and Presenter: Dmitry **Savostyanov** (University of Brighton, UK)

Co-author: Sergey **Dolgov** (University of Bath, UK)

Abstract

High-dimensional integrals appear in problems with uncertainty and noise and are common in stochastic calculus, mathematical finance, quantum physics, etc. Textbook quadratures applied to d-dimensional integrals require exponential in d number of function evaluations, which is unfeasible for dimensions exceeding ten (this is notoriously known as curse of dimensionality). The use of Smolyaks sparse grids relaxes, but does not completely remove the problem. Currently such integrals are predominantly treated with Monte Carlo algorithm or its variants, e.g. quasi-MC, MCMC, but their relatively slow convergence leads to excessive numerical costs and sometimes limits the accuracy of results.

Can we do better by using more structure of the original problem? We propose a new algorithm which interpolates the given function with a low-rank tensor product format using separation of variables. Our method is based on adaptive cross interpolation and maximum-volume principle – well-established algorithms for matrices, which we generalised to high-dimensional tensors [1]. To be competitive with Monte Carlo, a parallel version of tensor interpolation algorithm is necessary, and it is presented in this talk.

We demonstrate the efficiency of the proposed algorithm for a class of Ising integrals, which appear in Ising theory of mathematical physics in relation to magnetic susceptibility of two-dimensional spin lattices. This application encourages evaluation of integrals in dimensions up to 1000 with very high precision. Monte Carlo methods are not up to the challenge. Using tensor low-rank interpolation we compute integrals accurately to 100 decimal digits [2].

We hope that this example encourages further study and exploitation of low-rank tensor product structure for problems in other subject areas where the curse of dimensionality stands in the way of delivering highly accurate results at reasonable cost.

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Learning high-dimensional additive models on the torus

Author and Presenter: Michael **Schmischke** (TU Chemnitz, Germany)

Co-author: Daniel **Potts** (TU Chemnitz, Germany)

Abstract

We consider high-dimensional 1-periodic functions $f\colon \mathbb{T}^d \to \mathbb{R}$, where $d \in \mathbb{N}$ is the spatial dimension. Any such function which is square-integrable, i.e., $f \in \mathrm{L}_2(\mathbb{T}^d)$, can be uniquely represented using the multivariate classical ANOVA (analysis of variance) decomposition $f = \sum_{\boldsymbol{u}\subseteq\mathcal{D}} f_{\boldsymbol{u}}$. Here, $\mathcal{D} = \{1, 2, \dots, d\}$ is the set of coordinate indices and $f_{\boldsymbol{u}}\colon \mathbb{T}^{|\boldsymbol{u}|} \to \mathbb{R}$ for $\boldsymbol{u} \subset \mathcal{D}$ is an ANOVA term. We study the ANOVA decomposition in the frequency domain and develop new high-dimensional approximation methods.

We investigate how f inherits its smoothness to the ANOVA terms for Sobolev type spaces $\mathrm{H}^w(\mathbb{T}^d) = \{f \in \mathrm{L}_2(\mathbb{T}^d)\colon \sum_{\boldsymbol{k}\in\mathbb{Z}^d} w^2(\boldsymbol{k})|\hat{f}_{\boldsymbol{k}}|^2 < \infty\}$ and the weighted Wiener algebra $\mathcal{A}^w(\mathbb{T}^d) = \{f \in \mathrm{L}_1(\mathbb{T}^d)\colon \sum_{\boldsymbol{k}\in\mathbb{Z}^d} w(\boldsymbol{k})|\hat{f}_{\boldsymbol{k}}| < \infty\}$. Moreover, we consider the truncated ANOVA decomposition

$$\mathrm{T}_{d_s} f = \sum_{\substack{\boldsymbol{u}\subseteq\mathcal{D}\\ |\boldsymbol{u}|\le d_s}} f_{\boldsymbol{u}} \tag{1}$$

with superposition dimension $1 \le d_s < d$ and derive error-bounds for approximation by $\mathrm{T}_{d_s} f$ in L_∞ and L_2.

In this talk, we present methods for approximation of a function f in two scenarios:

- We have black-box-access to the function f.
- Only scattered data is available, i.e., a finite node set $X \subseteq \mathbb{T}^d$ and evaluations $\boldsymbol{y} = (f(\boldsymbol{x}))_{x\in X}$.

In both scenarios, we use (1) as approximation model and aim to rank the importance of the ANOVA terms $f_{\boldsymbol{u}}$, $|\boldsymbol{u}| \le d_s$, in order to construct a frequency index set $I \subseteq \mathbb{Z}^d$ for approximation of f by the corresponding Fourier partial sum

$$f(\boldsymbol{x}) \approx \mathrm{T}_{d_s} f(\boldsymbol{x}) \approx \sum_{\boldsymbol{k}\in I} \hat{f}_{\boldsymbol{k}} \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k}\cdot\boldsymbol{x}}.$$

We present methods for recovering the Fourier coefficients $\hat{f}_{\boldsymbol{k}}$ of f in both scenarios. In the black-box case, we rely on rank-1 lattice as sampling schemes and employ the lattice FFT. For scattered data, we iteratively solve a least-squares problem while using the non-equispaced FFT for efficient multiplication with the arising Fourier matrices.

Kernel-based lattice point interpolation for UQ using periodic random variables

Author and Presenter: Ian **Sloan** (University of New South Wales, Australia)

Co-authors: Vesa **Kaarnio ja** (University of New South Wales, Australia)
Yoshihito **Kazashi** (EPFL, Switzerland)
Frances **Kuo** (University of New South Wales, Australia)
Fabio **Nobile** (EPFL, Switzerland)

Abstract

This talk describes a kernel-based approximation method based on lattice points, for the approximate solution of an elliptic PDE with an input random field described by periodic stochastic variables. The analysis (incorporating results obtained recently by Cools, Kuo, Nuyens and Sloan) shows that with well chosen lattice points the method can give the best possible rate of L_2 convergence for any method that uses lattice points, and a manageable error bound even if the stochastic dimension is high. The practical advantage of the method is that the lattice structure makes it simple and cheap to implement: the $N \times N$ kernel matrix is a circulant matrix, and so has only N different elements, while being easily inverted by Fast Fourier Transform; and the kernel is available in closed form even when the dimension d is large, and computable in a time of order d.

Deterministic and probabilistic point sets on the unit sphere

Author and Presenter: Tetiana **Stepaniuk** (RICAM, Austria)

Abstract

We make a comparison between certain probabilistic (with respect to jittered samplings) and deterministic point sets (spherical t-designs, minimizing point-sets). Also we found the asymptotic equalities for the discrete Riesz s-energy and logarithmic energy of N-point sequence of well separated t-designs on the unit sphere $\mathbb{S}^d \subset \mathbb{R}^{d+1}$, $d \geq 2$. It is shown that asymptotically some deterministic constructions are better or as good as probabilistic ones.

For the classical Sobolev spaces $\mathbb{H}^s(\mathbb{S}^d)$ $(s > \frac{d}{2})$ upper and lower bounds for the worst case integration error of numerical integration on the unit sphere $\mathbb{S}^d \subset \mathbb{R}^{d+1}$, $d \geq 2$, have been obtained by Brauchart, Hesse and Sloan. We investigate the case when $s \to \frac{d}{2}$ and introduce the spaces $\mathbb{H}^{\frac{d}{2},\gamma}(\mathbb{S}^d)$ of continuous functions on $\mathbb{S}^d$ with an extra logarithmic weight. For these spaces we obtain estimates for the worst case integration error.

Lattice rules for integration over $\mathbb{R}^d$

Author and Presenter: Yuya **Suzuki** (KU Leuven, Belgium)

Co-author: Dirk **Nuyens** (KU Leuven, Belgium)

Abstract

In this talk, we consider numerical integration over $\mathbb{R}^d$ using lattice rules. For integration over the (unit) cube it is known that tent-transformed lattice rules can achieve up to second order convergence in a non-periodic unanchored Sobolev space [1, 2]. We show if it is possible to obtain higher order convergence, including truncation error, in an unanchored Sobolev space using lattice rules for integration over $\mathbb{R}^d$. We make use of an orthogonal projection from an unanchored Sobolev space to a Korobov space. Using this projection we can measure/quantify the non-periodicity of a function, and by imposing some decay condition on the integrand we achieve higher order. We also mention some complementary results using this projection.

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Convergence order of Euler-type schemes for SDEs in mathematical finance

Author and Presenter: Michaela **Szölgyenyi** (University of Klagenfurt, Austria)

Co-authors: Andreas **Neuenkirch** (University of Mannheim, Germany)
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Abstract

Stochastic differential equations (SDEs) are essential for many models mathematical finance. In many cases the coefficients of these SDEs lack regularity properties that are assumed in the classical literature on numerical methods for SDEs. For example when solving stochastic control problems in mathematical finance by simulation one has to take into account that the control might depend on the controlled process in an irregular (non-Lipschitz) manner. Motivated by this problem we study the strong convergence rate of the Euler-Maruyama scheme for scalar SDEs with additive noise and irregular drift. We provide a framework for the error analysis by reducing it to a weighted quadrature problem for irregular functions of Brownian motion. By analysing the quadrature problem we obtain for arbitrarily small $\epsilon > 0$ a strong convergence order of $(1 + \kappa)/2 - \epsilon$ for a non-equidistant Euler-Maruyama scheme, if the drift has Sobolev-Slobodeckij-type regularity of order κ.

In the multi-dimensional setting we allow the drift coefficient to be non-Lipschitz on a set of positive reach. We prove strong convergence of an Euler-type scheme, which uses adaptive step-sizing for a better resolution close to the discontinuity. We obtain a numerical method which has – up to logarithmic terms – strong convergence order $1/2$ with respect to the average computational cost, which is the best we can expect.

Optimally weighted nonlinear least-squares

Author and Presenter: Philipp **Trunschke** (Technische Universität Berlin, Germany)

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Reinhold **Schneider** (Technische Universität Berlin, Germany)

Abstract

We consider best approximation problems in a (nonlinear) subspace $\mathcal{M}$ of a Banach space $(\mathcal{V}, \|\bullet\|)$ where only an empirical estimate $\|\bullet\|_n$ of the norm can be computed. The norm is assumed to be of the form $\|v\| := \mathbb{E}_Y[|v|_Y^2]^{1/2}$ for some (parametric) semi-norm $|\bullet|_Y$ and some random variable Y. The objective is to approximate an unknown function $u \in \mathcal{V}$ by $v \in \mathcal{M}$, minimizing the empirical norm $\|u - v\|_n^2 := \frac{1}{n}\sum_{i=1}^n |u - v|_{y_i}^2$ w.r.t. n random samples $\{y_i\}_{i=1,\dots,n}$. It is common knowledge that such generalized least squares approximations can become inaccurate and unstable when the number of samples n is too close to the number of parameters $m := \dim(\mathcal{M})$. We review this statement in the light of adapted distributions for the samples y_i and establish a restricted isometry property (RIP) $(1-\delta)\|v\| \leq \|v\|_n \leq (1+\delta)\|v\|$ $\forall v \in \mathcal{M}$ which holds in probability. This RIP is then utilized to prove error bounds for the empirical best approximation problem. These results are closely related to those of Cohen and Migliorati [SMAI Journal of Computational Mathematics, 3, 181 (2017)] and show that, with high probability, $n \geq sm$ is sufficient for the RIP to be satisfied, with the factor s representing the variation of the empirical norm $\|\bullet\|_n$ on $\mathcal{M}$. Finally, we apply the theory to a well-known benchmark problem in uncertainty quantification and provide numerical examples for some of the theoretical predictions.

Random rank-1 lattices and high-dimensional sparse FFT

Author and Presenter: Toni **Volkmer** (TU Chemnitz, Germany)

Co-authors: Lutz **Kämmerer** (TU Chemnitz, Germany)
Felix **Krahmer** (TU München, Germany)

Abstract

Sampling schemes based on so-called rank-1 lattices allow for powerful methods for numerical integration and reconstruction of high-dimensional periodic functions. In order to efficiently reconstruct such functions, they should fulfill certain properties like special smoothness characteristics or (approximate) sparsity in frequency domain. Then, they can be well approximated by multivariate trigonometric polynomials consisting only of a relatively small number of oscillations with certain frequencies and corresponding Fourier coefficients. The hard task is determining the (often) unknown frequencies in a fast way using as few measurements of the function under consideration as possible. In one spatial dimension, several methods called sparse fast Fourier transform (sparse FFT) are available for solving this task. However, the high-dimensional case is much more challenging, especially if the number of possible frequencies, i.e. the cardinality of the search space, is very huge.

In this talk, new results on high-dimensional sparse FFT are presented, which use a recently developed sampling scheme called "random rank-1 lattices". This sampling method distinctly improves the required number of samples compared to the approach in [1]. The idea behind "random rank-1 lattices" is explained and theoretical results are presented.

Two approaches for the reconstruction of high-dimensional periodic functions based on "random rank-1 lattices" are discussed. The first approach utilizes a direct search for the frequencies belonging to the approximately largest Fourier coefficients. The number of samples only depends logarithmically on the number of possible frequencies and the arithmetic complexity only linearly. The second approach provides additional improvements for the case where the number of possible frequencies is extremely huge. Then, we propose to use a search method based on dimension-incremental projections from [1] using "random rank-1 lattices", which distinctly reduces the arithmetic complexity. The talk is concluded by presenting impressive numerical results for up to 30 spatial dimensions.

References

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On the Dependence Structure of Scrambled (t, m, s)-nets

Author and Presenter: Jaspar **Wiart** (RICAM, Austria)

Co-author: Christiane **Lemieux** (University of Waterloo, Canada)

Abstract

We study the dependence structure of scrambled (t, m, s)-nets and show that they have a negative lower/upper orthant dependence structure if and only if $t = 0$. This study allows us to gain a deeper understanding about the classes of functions for which the variance of estimators based on scrambled $(0, m, s)$-nets can be proved to be no larger than that of a Monte Carlo estimator.

Better approximations of high dimensional smooth functions by deep neural networks with rectified power units

Author and Presenter: Haijun **Yu** (Academy of Math. & Systems Sci., CAS, China)

Co-authors: Bo **Li** (Academy of Math. & Systems Sci., CAS, China)
Shanshan **Tang** (Academy of Math. & Systems Sci., CAS, China)

Abstract

Deep neural networks with rectified linear units (ReLU) are recently getting very popular due to its universal representation power and easier to train. Some theoretical progresses on deep ReLU network approximation power for functions in Sobolev space and Korobov space have recently been made by several groups. In this talk, we show that deep networks with rectified power units (RePU) can give better approximations for smooth functions than deep ReLU networks. Our analyses base on classical polynomial approximation theory and some efficient algorithms we proposed to convert polynomials into deep RePU networks of optimal size without any approximation error. Our constructive proofs reveal clearly the relation between the depth of the RePU network and the order of polynomial approximation. Taking into account some other good properties of RePU networks, such as being high-order differentiable, we advocate the use of deep RePU networks for problems where the underlying high dimensional functions are smooth or derivatives are involved in the loss function.

Multi-fidelity machine learning by the sparse grid combination technique

Author and Presenter: Peter **Zaspel** (University of Basel, Switzerland)

Abstract

The solution of parametric partial differential equations or other parametric problems is the main component of many applications in scientific computing. Such applications include, but are not limited to, uncertainty quantification, inverse problems and optimization. To avoid the re-implementation of scientific simulation codes, the use of snapshot-based (non-intrusive) techniques for the solution of parametric problems becomes very attractive.

In this presentation, I will report on ongoing work to solve parametric problems with a higher-dimensional parameter space by means of approximation in reproducing kernel Hilbert spaces. In presence of regularization, approximation in reproducing kernel Hilbert spaces is equivalent to the so-called "kernel ridge regression", which is a classical approach in machine learning. In that sense, results on the use of machine learning for an efficient approximation of parametric problems will be discussed.

One challenge in parametric problems with high-dimensional parameter space is the high number of simulation snapshots that has to be computed in order to get a low approximation error with respect to the parameter space. If a single simulation is computationally expensive, many simulations of this kind become computationally intractable. To overcome this, we have introduced a multi-fidelity kernel ridge regression approach based on the sparse grid combination technique or multi-index approximation. In fact, this approach allows to significantly reduce the number of expensive calculations by adding coarser and coarser simulation snapshots.

The results presented in this talk include applications in quantum chemistry [1] and computational fluid mechanics [2] and are based in parts on joined work with Michael Griebel, Helmut Harbrecht, Bing Huang, Christian Rieger and Anatole von Lilienfeld (in alphabetical order).

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A ResNet-based isosurface learning method for dimensionality reduction in high-dimensional function approximation

Author and Presenter: Guannan **Zhang** (Oak Ridge National Laboratory, USA)

Co-author: Jacob **Hinkle** (Oak Ridge National Laboratory, USA)

Abstract

We developed a ResNet-based iso-surface learning method for dimensionality reduction in high-dimensional function approximation. Existing linear methods, including sliced inverse regression, active subspace methods, reduce the dimensionality by imposing a ridge function structure and learning an affine/linear transformation; and our contribution is to extend such transformation to the nonlinear regime. Specifically, we defined a nonlinear transformation using one type of reversible ResNets, and trained the ResNets to approximately parametrize the target function's iso-surfaces in low-dimensional parameter spaces, so as to greatly increase the anisotropy of the transformed function. A new loss function was designed for training the ResNets, such that the trained transformation can approximately capture the nonlinearity of the iso-surface. The effectiveness of our approach is demonstrated by applying it to three two-dimensional functions for illustrating the nonlinearity of the transformation, as well as to several twenty-dimensional functions for showing the improved approximation accuracy with the use of the nonlinear transformation.

A neural network based policy iteration algorithm with global H^2-superlinear convergence for stochastic games on domains

Author and Presenter: Yufei **Zhang** (University of Oxford, UK)

Co-authors: Kazufumi **Ito** (North Carolina State University, USA)
Christoph **Reisinger** (University of Oxford, UK)

Abstract

In this work, we propose a class of numerical schemes for solving semilinear Hamilton-Jacobi-Bellman-Isaacs (HJBI) boundary value problems which arise naturally from exit time problems of diffusion processes with controlled drift. We exploit policy iteration to reduce the semilinear problem into a sequence of linear Dirichlet problems, which are subsequently approximated by a multilayer feedforward neural network ansatz. We establish that the numerical solutions converge globally in the H^2-norm, and further demonstrate that this convergence is superlinear, by interpreting the algorithm as an inexact Newton iteration for the HJBI equation. Moreover, we construct the optimal feedback controls from the numerical value functions and deduce convergence. The numerical schemes and convergence results are then extended to oblique derivative boundary conditions. Numerical experiments on the stochastic Zermelo navigation problem and the perpetual American option pricing problems are presented to illustrate the theoretical results and to demonstrate the effectiveness of the method.

References

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Sparse polynomial interpolation and symmetric tensor decomposition

Author and Presenter: Lihong **Zhi** (Academy of Math. and Systems Sci., Beijing, China)

Abstract

The sparse interpolation problem has been studied and widely used in many different areas of science and engineering since the work of Prony (1795). Ankur Moitra in his paper at STOC 2015 has given an in-depth analysis of how oversampling improves the conditioning of the arising Prony systems for sparse interpolation and signal recovery from numeric data. Moitra assumes that oversampling is done for a number of samples beyond the actual sparsity of the polynomial/signal. We give an algorithm that can be used to compute the sparsity and estimate the minimal number of samples needed in numerical sparse interpolation. Some recent work on computing the symmetric tensor rank by Pronys method will also be introduced.

Constructing least-squares multivariate polynomial approximation

Author and Presenter: Tao **Zhou** (Chinese Academy of Sciences, China)

Co-authors: John **Jakeman** (Sandia Lab, USA)
Akil **Narayan** (University of Utah, USA)

Abstract

Polynomial approximations constructed using a least squares approach is a ubiquitous technique in numerical computations. One of the simplest ways to generate data for the least squares problems is with random sampling of a function. We discuss theory and algorithms for stability of the least-squares problem using random samples. The main lesson from our discussion is that the intuitively straightforward ("standard") density for sampling frequently yields suboptimal approximations, whereas sampling from a non-standard density either by the so-called induced distribution or the asymptotic equilibrium measure, yields near-optimal approximations. We present recent theory that demonstrates why sampling from such measures is optimal, and provide several computational experiments that support the theory. New applications of the equilibrium measure sampling will also be discussed.

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