

Institute for Numerical Simulation

Rheinische Friedrich-Wilhelms-Universität Bonn

10^{th} Workshop on HIGH-DIMENSIONAL APPROXIMATION

BOOK OF ABSTRACTS

DATE: Location:	2025/09/08 – 2025/09/12 Bonn, Germany				
Program Committee:	Ben Adcock (Simon Fraser University, Canada) Markus Bachmayr (RWTH Aachen, Germany) Santiago Badia (Monash University, Australia) Albert Cohen (Sorbonne Université, France) Jochen Garcke (U Bonn & Fraunhofer SCAI, Germany) Michael Griebel (U Bonn & Fraunhofer SCAI, Germany) Markus Hegland (ANU, Australia) Fred Hickernell (Illinois Institute of Technology, USA) George Em Karniadakis (Brown University, USA) Frances Kuo (UNSW, Australia) Christiane Lemieux (University of Waterloo, Canada) Fabio Nobile (ÉPF Lausanne, Switzerland) James Nichols (ANU, Australia) Ian Sloan (UNSW, Australia) Tino Ullrich (TU Chemnitz, Germany) Dingxuan Zhou (University of Sydney, Australia)				
LOCAL ORGANIZERS:	Bastian Bohn (University of Bonn, Germany)				
Contact:	http://ins.uni-bonn.de/2025/hda mailto:hda2025@ins.uni-bonn.de				
Sponsors:	Hausdorff Center for Mathematics University of Bonn – TRA Modelling CRC1639 NuMeriQS				



FRIEDRICH-WILHELMS- RESEARCH AREA UNIVERSITÄT BONN

RHEINISCHE TRANSDISCIPLINARY



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General Information

The High-Dimensional Approximation (HDA) Workshop is a series of biennial international meetings covering current research on high-dimensional problems.

The 10th Workshop on High-Dimensional Approximation covers a range of topics central to modern high-dimensional approximation and their applications. The scope ranges from high-dimensional approximation theory over computational methods to engineering and scientific applications.

This international workshop is the tenth in a series which were previously held at The Australian National University in Canberra (HDA 2005, HDA 2007, HDA 2013, and HDA 2023), at the University of New South Wales in Sydney (HDA 2009 and HDA 2017), at the ETH Zurich (HDA 2019), and at the University of Bonn (HDA 2011 and HDA 2015).

This year the workshop returns to University of Bonn to be held from September, $08^{\text{th}} - 12^{\text{th}}$, 2025.

Venue

The workshop takes place at the

Universitätsclub Bonn, Konviktstraße 9, 53115 Bonn, https://uniclub-bonn.de.

We will have a data-projector, a flipchart and laptops with Acrobat-Reader in the conference room. Please bring your talk (.pdf) along with you on a USB-stick. If you need any other hard- or software (e.g. video adapter cable for your own MacBook) to present your talk, please make sure to bring them yourself. Network access (WLAN) for reading email, etc. is available throughout the university club.

Workshop beginning

We will start with lunch on Monday, September 08th, at 12:30 p.m. Our registration desk will also open at the same time. Before and after the workshop, you can contact us by email at hda2025@ins.uni-bonn.de.

Icebreaker Reception

Sunday, 2025/09/07, 1900: Icebreaker Reception in the local brewery "Bönnsch", Sterntorbrücke 4, 53111 Bonn, https://www.boennsch.de. It is in the direct vicinity of the bus stop "Friedensplatz" and of the bus and tram stop "Stadthaus".

Please inform us at hda2025@ins.uni-bonn.de until September, 5th, if you want to join.

Conference Dinner

Thursday, 2025/09/11, 1900: Conference Dinner in the "Gasthaus im Stiefel", Bonngasse 30, 53111 Bonn, https://www.gasthausimstiefel.de.

It is approximately a 10 minute footwalk from the university club to the Gasthaus im Stiefel. It can also easily be reached via the bus and tram station "Bertha-von-Suttner-Platz/Beethovenhaus".



Invited Speakers

For this year's Workshop on High-Dimensional Approximation

- Sergey Dolgov (University of Bath, UK)
- Omar Ghattas (The University of Texas at Austin, USA)
- Takashi Goda (The University of Tokyo, Japan)
- Fred J. Hickernell (Illinois Institute of Technology, USA)
- Gitta Kutyniok (Ludwig Maximilian University of Munich, Germany)
- Benjamin Peherstorfer (New York University, USA)
- Peter Richtárik (King Abdullah University of Science and Technology, Kingdom of Saudi Arabia)
- Ian Sloan (University of New South Wales, Australia)
- Michaël Unser (École Polytechnique Fédérale de Lausanne, Switzerland)

were invited by the Hausdorff Center for Mathematics and the Institute for Numerical Simulation at the University of Bonn to give an extended 40-minute talk.

Program Committee

- Ben Adcock (Simon Fraser University, Canada)
- Markus Bachmayr (RWTH Aachen, Germany)
- Santiago Badia (Monash University, Australia)
- Albert Cohen (Sorbonne Université, France)
- Jochen Garcke (U Bonn & Fraunhofer SCAI, Germany)
- Michael Griebel (U Bonn & Fraunhofer SCAI, Germany)
- Markus Hegland (ANU, Australia)
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- James Nichols (ANU, Australia)
- Ian Sloan (UNSW, Australia)
- Tino Ullrich (TU Chemnitz, Germany)
- Dingxuan Zhou (University of Sydney, Australia)

Local Organizers

• Bastian Bohn (University of Bonn, Germany)

Sponsors

The workshop is hosted by the

Institute for Numerical Simulation, University of Bonn, http://www.ins.uni-bonn.de,

in cooperation with the

Hausdorff Center for Mathematics, University of Bonn, http://www.hcm.uni-bonn.de,

 ${\rm the}$

Transdisciplinary Research Area Modelling, University of Bonn, https://www.uni-bonn.de/en/research-and-teaching/research-profile/ transdisciplinary-research-areas/tra-1-modelling

and the

Collaborative Research Centre 1639 NuMeriQS, University of Bonn, https://numeriqs.hiskp.uni-bonn.de.

We are grateful for the financial support of those sponsors.

Timetable

Time	Monday 08th	Tuesday 09th	Wednesday 10th	Thursday 11th	Friday 12th		
09:00-09:30		M. Fernandes	T. Lê	P. Kritzer	HJ. Flad		
09:30-10:00		J. Schmidt	M. Schmidlin	D. Nuyens	D. Dinh		
10:00-10:30		J. von Smercek	AA. Zepernick	Y. Zhou	H. Eisenmann		
10:30-11:00		Coffee Break					
11:00-11:40		G. Kutyniok	T. Goda	O. Ghattas	B. Peherstorfer		
11:40-12:10		H. Wendland	Y. Kazashi	G. Maier	H. Yang		
12:10-12:40		R. Kempf	M. Gnewuch	R. von Rickenbach	Closing remarks		
12:40-13:50	Lunch [until 13:30] Welcome [at 13:30]	Lunch Buffet					
13:50-14:20	C. Miranda	A. Little	F. Bartel	J. Dölz			
14:20-14:50	Y. Cheng	S. Mishra	A. Gilbert	Y. Suzuki			
14:50-15:30	S. Dolgov	M. Unser	I. Sloan	P. Richtárik			
15:30-16:00		Coffee					
16:00-16:30	J. Heieck	J. Teichmann	16:00 – 16:40 F. Hickernell	A. Zeiser			
16:30-17:00	G. Li	P. Zaspel	16:40 – 17:10 Z. Pan	J. Garcke			
17:00-17:30	P. Roy	M. Wnuk		R. Khotyachuk			
17:30-19:00							
19:00-21:00				Workshop Dinner			

Detailed Program

Monday, September 08th, 2025

13:50–14:20, Charles Miranda. Properties and optimisation of compositional tensor networks.

14:20–14:50, Yingda Cheng. Low-rank Anderson Acceleration.

14:50–15:30, Sergey Dolgov. Deep tensor train approximation of transport maps for Bayesian inverse problems.

16:00–16:30, Jacob Heieck. Lyapunov Stability of Consensus-Based Optimization.

16:30–17:00, Guanglian Li. Gradient-enhanced sparse Hermite polynomial expansions for pricing and hedging high-dimensional American options.

17:00–17:30, Priyanka Roy. Gradient Descent Algorithm in Hilbert Spaces under Stationary Markov Chains with ϕ - and β -Mixing.

Tuesday, September 09th, 2025

09:00–09:30, Matthew Fernandes. Surrogate Bayesian Inversion for a Class of Wave Configuration Parameters.

09:30–10:00, Johannes Schmidt. Sparse Grid for Multi-Level Combination Methods in Machine Learning.

10:00–10:30, Julius von Smercek. Gradient-Based Adaptive Refinement on Sparse Grids for Critical Event Estimation.

11:00–11:40, Gitta Kutyniok. *tba*.

11:40–12:10, Holger Wendland. Kernel-based approximation of high-dimensional functions with small efficient dimension.

12:10–12:40, Rüdiger Kempf. Revisiting the Tensor Product Multilevel Method: New Insights into Kernel-Based Sparse Grid Approximation.

13:50–14:20, Anna Little. Functional Multi-Reference Alignment via Deconvolution.

14:20–14:50, Shiv Mishra. Consistent PINNs for parabolic PDEs.

14:50–15:30, Michael Unser. tba.

16:00–16:30, Josef Teichmann. Path dependent time series models.

16:30–17:00, Peter Zaspel. Data-driven identification of port-Hamiltonian DAE systems by Gaussian processes.

17:00–17:30, Marcin Wnuk. Adaptive and non-adaptive approximation of high-dimensional vectors.

Wednesday, September 10th, 2025

09:00–09:30, Tùng Lê. *Quasi-Monte-Carlo method for Gevrey class functions governed by non-linear PDEs.*

09:30–10:00, Marc Schmidlin. A framework for proving parametric regularity of high-dimensional problems.

10:00–10:30, André-Alexander Zepernick. Domain UQ for stationary and time-dependent PDEs using QMC.

11:00–11:40, Takashi Goda. Quasi-uniform quasi-Monte Carlo point sets and sequences.

11:40–12:10, Yoshihito Kazashi. (Near-)Optimality of Quasi-Monte Carlo methods and Suboptimality of the Sparse-Grid Gauss-Hermite Rule in Gaussian Sobolev Spaces.

12:10–12:40, Michael Gnewuch. Data Compression using Rank-1 Lattices for Parameter Estimation in Machine Learning.

13:50–14:20, Felix Bartel. Minimal Subsampled Rank-1 Lattices for Multivariate Approximation with Optimal Convergence Rate.

14:20–14:50, Alexander Gilbert. A novel CBC construction for lattice rules for L^2 approximation with POD and SPOD weights.

14:50–15:30, Ian Sloan. tba.

16:00–16:40, Fred Hickernell. The Quality of Lattice and Kronecker Sequences.

16:40–17:10, Zexin Pan. Dimension-independent convergence rates of median randomized nets.

Thursday, September 11th, 2025

09:00-09:30, Peter Kritzer. Median lattice rules for function approximation.

09:30–10:00, Dirk Nuyens. Least squares using Kronecker points.

10:00–10:30, Yiqing Zhou. Minimization of Costly Functions Using Sparse FFT-Based Interpolation.

11:00-11:40, Omar Ghattas. tba.

11:40–12:10, Gregor Maier. Near-Optimal Learning of Lipschitz Operators with respect to Gaussian Measures.

12:10–12:40, Remo von Rickenbach. On Sobolev and Besov Spaces With Hybrid Regularity.

13:50–14:20, Jürgen Dölz. Uncertainty quantification of spectral clusterings.

14:20–14:50, Yuya Suzuki. Approximations of Differential Entropy in Bayesian Optimal Experimental Design

14:50–15:30, Peter Richtárik. tba.

16:00–16:30, Andreas Zeiser. Discontinuous Galerkin discretization of conservative dynamical low-rank approximation schemes for the Vlasov-Poisson equation.

16:30–17:00, Jochen Garcke. tba.

17:00–17:30, Roman Khotyachuk. Dimensionality reduction techniques for numerical solutions of the Elder problem.

Friday, September 12th, 2025

09:00-09:30, Heinz-Jürgen Flad. Higher Order Singularities in High Dimensions.

09:30–10:00, Dinh Dũng. Sampling recovery in Bochner spaces and applications to parametric PDEs with random inputs.

10:00–10:30, Henrik Eisenmann. Optimal solvers for infinite-dimensional sparse approximations in adaptive stochastic Galerkin finite element methods.

11:00–11:40, Benjamin Peherstorfer. *DICE: Discrete inverse continuity equation for learning population dynamics.*

11:40–12:10, Huqing Yang. Sparse and low-rank approximations of parametric PDEs: the best of both worlds.

Properties and optimisation of compositional tensor networks

Eigel, M.¹, Miranda, C.², Nouy, A.², and Sommer, D.¹

¹Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany ²Centrale Nantes, Nantes Université, Laboratoire de Mathématiques Jean Leray UMR CNRS 6629, France

Abstract

In this work, we introduce compositional tensor networks (CTN), as a new approximation format merging the strengths of low-rank tensor formats and neural networks. Tensor networks have gained prominence in high-dimensional data analysis and functional approximation, particularly for their robustness and computational efficiency. Neural networks, while more powerful, often require extensive resources and time for training. CTNs combine the benefits of both approaches. We also propose a training procedure for this architecture based on the natural gradient descent. The natural gradient is known for being invariant under reparameterization and for aligning with the true functional gradient under an appropriate metric. This frequently leads to faster and more stable convergence compared to standard Euclidean-gradient-based optimization. Although computing the natural gradient is generally intractable in high-dimensional settings, we show that in the CTN context, it can be computed efficiently using tensor algebra. Moreover, the structure of CTNs allows the use of low-rank constraints during training, further improving computational scalability. The efficiency of this approach is illustrated on benchmark problems in regression.

Low-rank Anderson Acceleration

Appelö, $D.^1$ and Cheng, $Y.^1$

¹Virginia Tech, USA

Abstract

We present the low-rank Anderson Acceleration (lrAA), a numerical method that directly computes low rank solutions to nonlinear equations. In many applications (e.g. nonlinear diffusion), the approximate solution, when represented as a matrix, is approximately low rank. It is challenging to design a numerical scheme for nonlinear equations that work directly with low rank. A principal challenge is that if nonlinearities are evaluated element-wise for all matrix elements then the computational savings, from quadratic to linear in the grid points per dimension, is lost.

We propose IrAA, which is based on Anderson Acceleration (AA), a well known technique for accelerating Picard iteration for fixed point problems. We couple AA with low rank truncation and cross approximations. We develop a new method for matrix cross approximation, Cross-DEIM, that uses the discrete empirical interpolation method (DEIM) based index selection to achieve effective cross approximations throughout the iterations. We show that IrAA works well for benchmark problems. We extend the method to higher dimensions in Tucker tensor format.

Deep tensor train approximation of transport maps for Bayesian inverse problems

Cui, T.¹, Dolgov, S.², and Scheichl, R.³

¹University of Sydney ²University of Bath ³University of Heidelberg

Abstract

Tensor networks (such as the tensor train decomposition) are efficient compression methods for multivariate tensors and discretized functions, provided that variables are locally correlated in some sense. However, this may be not the case for many practically relevant functions, such as the posterior probability density functions in Bayesian inverse problems. We develop a deep transport map to decorrelate the variables by transforming the distribution, which density is defined by a simplification of the given function, to the uniform distribution [1]. In turn, each simplified function is approximated by the tensor train decomposition. We introduce a sequence of function simplifications and the corresponding composition of the transport maps such that each function admits an efficient tensor train approximation. We propose two strategies for this simplifying sequence: tempering of the target density [1], and smoothing of an indicator function with sigmoid functions of varying scale [2]. The latter opens the door to efficient computation of hitherto unattainable rare event probabilities in Bayesian inference problems.

- T. Cui and S. Dolgov. "Deep Composition of Tensor-Trains Using Squared Inverse Rosenblatt Transports". In: Found. Comput. Math. 22.6 (2022), pp. 1863–1922. DOI: 10.1007/s10208-021-09537-5.
- [2] Tiangang Cui, Sergey Dolgov, and Robert Scheichl. "Deep Importance Sampling Using Tensor Trains with Application to a Priori and a Posteriori Rare Events". In: SIAM Journal on Scientific Computing 46.1 (2024), pp. C1–C29. DOI: 10.1137/23M1546981.

Lyapunov Stability of Consensus-Based Optimization

Heieck, J.¹, Göttlich, S.¹, and Neuenkirch, A.¹

¹University of Mannheim

Abstract

We study the finite-agent behavior of Consensus-Based Optimization (CBO), a recent metaheuristic for the global minimization of a function, that combines drift toward a consensus estimate with stochastic exploration. While previous analyses focus on asymptotic mean-field limits, we investigate the stability properties of CBO for finite population size N. Using a hierarchical approach, we analyze three increasingly complex systems: a purely deterministic model, a stochastic perturbation within a deterministic framework, and the full stochastic differential equation. Our results demonstrate that key stability properties persist across all settings.

Gradient-enhanced sparse Hermite polynomial expansions for pricing and hedging high-dimensional American options

Yang, $\mathrm{J.^1}$ and Li, $\mathrm{G.^2}$

^{1,2}The University of Hong Kong

Abstract

We propose an efficient and easy-to-implement gradient-enhanced least squares Monte Carlo method for computing price and Greeks (i.e., derivatives of the price function) of high-dimensional American options. It employs the sparse Hermite polynomial expansion as a surrogate model for the continuation value function, and essentially exploits the fast evaluation of gradients. The expansion coefficients are computed by solving a linear least squares problem that is enhanced by gradient information of simulated paths. We analyze the convergence of the proposed method, and establish an error estimate in terms of the best approximation error in the weighted H^1 space, the statistical error of solving discrete least squares problems, and the time step size. We present comprehensive numerical experiments to illustrate the performance of the proposed method. The results show that it outperforms the state-of-the-art least squares Monte Carlo method with more accurate price, Greeks, and optimal exercise strategies in high dimensions but with nearly identical computational cost, and it can deliver comparable results with recent neural network-based methods up to dimension 100.

Gradient Descent Algorithm in Hilbert Spaces under Stationary Markov Chains with ϕ - and β -Mixing

Roy, P.¹ and Saminger-Platz, S.¹

¹Institute for Mathematical Methods in Medicine and Data-Based Modeling, Johannes Kepler University Linz, Altenberger Strasse 69, A-4020 Linz, Austria

Abstract

In this contribution, we discuss a strictly stationary Markov chain gradient descent algorithm operating in general Hilbert spaces. We assume that the decay of dependence in the chain is characterized by ϕ - and β -mixing coefficients. Under these assumptions, we show probabilistic upper bounds on the convergence behavior of the algorithm based on the exponential as well as the polynomial decay of the mixing coefficients. Under exponential decay of both ϕ - and β -mixing coefficients, for $\theta \in (\frac{1}{2}, 1)$, the convergence rate remains $\mathcal{O}\left(t^{-\theta/2}\right)$, aligning with the i.i.d. rates established by Smale and Yao [1]. However, at the boundary case $\theta = 1$, the rate deteriorates to $\mathcal{O}\left(t^{-\alpha/2}\right)$, in contrast to the i.i.d. setting where a faster rate $\mathcal{O}\left(t^{-\alpha}\right)$ is achieved, as shown by Smale and Yao [1], where $\alpha \in (0, 1]$. As for the polynomial decay of both the mixing coefficients, for example, when $\phi_i \leq bi^{-k}$, where b > 0and k > 0, and parameter values $\theta \in \left(\frac{1}{2}, 1\right)$, the convergence rate remains the same as that of the i.i.d. rate for the value k > 1, however for k = 1, the rate is almost the same as that of the i.i.d. rate except for a logarithmic factor, i.e., $O\left(t^{-\theta/2}(\log t)^{1/2}\right)$. Moreover, we demonstrate that our results are sharp in the sense that when the mixing rate is fast, the dependence becomes negligible, making the error bounds and learning rates nearly identical to those observed for independent samples.

We further highlight the advantages of analyzing gradient descent algorithms within general Hilbert spaces by discussing their extension to online regularized learning algorithms, particularly in reproducing kernel Hilbert spaces. Specifically, we shall demonstrate how the error bounds and convergence rates derived for gradient descent algorithms driven by strictly stationary Markov chains in general Hilbert spaces can be adapted to the context of online regularized learning in RKHS, under assumptions involving ϕ - and β -mixing.

Note that in the above context, mixing coefficients have been a relevant measure of dependence in order to study various aspects of learning theory earlier; for example, Meir [2] extended the Vapnik-Chervonenkis framework to β -mixing time series, and Zou and Li [3] established convergence bounds for the empirical risk minization learning paradigm with an exponentially strongly mixing sequence. Subsequent works expanded the analysis via Rademacher complexity and stability bounds, notably by Mohri and Rostamizadeh [4, 5], for both β - and ϕ -mixing sequences. PAC-Bayes bounds under β - and ϕ -mixing were studied by Ralaivola [6]. Regarding regularization schemes, Xu and Chen [7] addressed the α -mixing setting, while Sun and Wu [8] considered both α - and ϕ -mixing sequences. Furthermore, SVM consistency and convergence rates under various mixing conditions were investigated by Steinwart *et al.* [9], Steinwart and Christmann [10], and Xu *et al.* [11]. More recently, Tong and Ng [12] analyzed spectral learning algorithms under strong mixing assumptions. In contrast to previous works, our contribution specifically investigate the performance of gradient descent algorithms for ϕ - and β -mixing strictly stationary Markov chains.

- Steve Smale and Yuan Yao. "Online learning algorithms". In: Found. Comput. Math. 6.2 (2006), pp. 145–170. ISSN: 1615-3375,1615-3383. DOI: 10.1007/s10208-004-0160-z.
- [2] Ron Meir. "Nonparametric time series prediction through adaptive model selection". In: *Machine learning* 39 (2000), pp. 5–34.
- [3] Bin Zou and Luoqing Li. "The performance bounds of learning machines based on exponentially strongly mixing sequences". In: Computers & Mathematics with Applications 53.7 (2007), pp. 1050– 1058.

- [4] Mehryar Mohri and Afshin Rostamizadeh. "Rademacher complexity bounds for non-iid processes". In: Advances in neural information processing systems 21 (2008).
- [5] Mehryar Mohri and Afshin Rostamizadeh. "Stability Bounds for Stationary φ -mixing and β -mixing Processes." In: Journal of Machine Learning Research 11.2 (2010).
- [6] Liva Ralaivola, Marie Szafranski, and Guillaume Stempfel. "Chromatic PAC-Bayes bounds for noniid data: Applications to ranking and stationary β -mixing processes". In: *The Journal of Machine Learning Research* 11 (2010), pp. 1927–1956.
- Yong-Li Xu and Di-Rong Chen. "Learning rates of regularized regression for exponentially strongly mixing sequence". In: J. Statist. Plann. Inference 138.7 (2008), pp. 2180–2189. ISSN: 0378-3758,1873-1171. DOI: 10.1016/j.jspi.2007.09.003.
- [8] Hongwei Sun and Qiang Wu. "Regularized least square regression with dependent samples". In: Adv. Comput. Math. 32.2 (2010), pp. 175–189. ISSN: 1019-7168,1572-9044. DOI: 10.1007/s10444-008-9099-y.
- [9] Ingo Steinwart, Don Hush, and Clint Scovel. "Learning from dependent observations". In: *Journal of Multivariate Analysis* 100.1 (2009), pp. 175–194.
- [10] Ingo Steinwart and Andreas Christmann. "Fast learning from non-iid observations". In: Advances in neural information processing systems 22 (2009).
- [11] Jie Xu et al. "Generalization performance of Gaussian kernels SVMC based on Markov sampling". In: Neural networks 53 (2014), pp. 40–51.
- [12] Hongzhi Tong and Michael Ng. "Spectral algorithms for learning with dependent observations". In: Journal of Computational and Applied Mathematics 437 (2024), p. 115437.

Surrogate Bayesian Inversion for a Class of Wave Configuration Parameters

Fernandes, M.J.¹, Ganesh, M.², and Hawkins, S.C.³

¹Macquarie University, Sydney, NSW, Australia ²Colorado School of Mines, Golden, CO, USA

Abstract

Using multiple scattering acoustic data from a given configuration, we develop and implement an efficient surrogate-based Bayesian inversion model to infer probabilistic posterior information about the unknown locations of several known scattering objects. The underlying stochastic wave propagation is modelled by the Helmholtz partial differential equation (PDE) in an unbounded domain surrounding the configuration, with the object locations treated as uncertain parameters. The available data consist of noisy far-field measurements generated by incident plane waves impinging on the configuration.

As the number of objects increases, the stochastic dimension of the problem grows, necessitating efficient sampling of the unnormalized Bayesian posterior distribution in a high-dimensional parameter space. Each posterior evaluation requires simulating the deterministic forward model—solving the Helmholtz PDE with boundary conditions defined by the one sample of object locations and their material properties. This process is computationally demanding due to the oscillatory nature of the solutions, which require fine discretization for accurate approximation.

To address this challenge, we introduce a surrogate model that significantly reduces computational cost. The surrogate exploits a decomposition of the solution into known highly oscillatory components and slowly varying residual terms, which are more amenable to efficient approximation. Numerical experiments confirm the surrogate's accuracy and demonstrate substantial gains in computational efficiency.

Sparse Grids for Multi-Level Combination Methods in Machine Learning

Schmidt, J.¹

¹Institut für Numerische Simulation, Universität Bonn, Friedrich-Hirzebruch-Allee 7, 53115 Bonn

Abstract

We investigate the use of sparse grid methods to improve computational efficiency in machine learning regression tasks. Our main goal is to explore whether the sparse grid combination technique can reduce training cost while maintaining predictive quality. Specifically, we consider model families $u_{\theta} \colon \mathbb{R}^{d} \to \mathbb{R}$ trained to minimize mean squared error on datasets of varying size and complexity.

To that end, we introduce a novel a posteriori approach that identifies a sparse grid structure across a two-dimensional hierarchy: one axis represents model complexity, the other the size of the training data. For each model in this grid, we estimate the trade-off between training cost and error reduction. If a beneficial pattern emerges—typically a diagonal decay in efficiency—we construct a combined model as a weighted sum of simpler models. This method is conceptually related to multifidelity techniques and naturally enables parallel training.

We demonstrate the approach on three types of regression problems: a synthetic 1D function, a real-world tabular dataset (Diabetes), and a high-dimensional image regression task (UTKFace). In all settings, the combined model achieves performance comparable to the most accurate individual models, at a fraction of the total training cost. In the CNN case, the benefit becomes particularly apparent at higher combination levels, though it depends on how the efficiency decays across the hierarchy.

These findings suggest that sparse grid combination is a promising strategy to scale regression tasks more efficiently. The method is flexible across model types and data domains and opens up new paths for adaptive and parallel learning architectures. While our current results are preliminary, they indicate the potential for significant speedups-by an order of magnitude for the CNN—without compromising performance.

Gradient-Based Adaptive Refinement on Sparse Grids for Critical Event Estimation

von Smercek, J¹, Baslan, N.^{1,2}, and Pflüger, D.¹

¹Scientific Computing, University of Stuttgart ²Search Based Testing, Bosch

Abstract

Risk analysis plays a crucial role in applications such as autonomous driving. Although critical driving situations are rare, they must be detected in advance and reliably excluded. Demonstrating that autonomous driving is as safe as human driving would require billions of kilometers to be driven [1]. This is practically infeasible and is therefore replaced by virtual driving in simulation. However, since simulations depend on numerous parameters, the curse of dimensionality also affects virtual experiments. Furthermore, each simulation is computationally intensive and costly. It is therefore essential to efficiently identify the parameter regions that lead to critical behavior.

We employ sparse grids with B-spline basis functions [3] to construct a surrogate of the objective function. Adaptive refinement enables a reduction in the number of expensive simulations. We propose novel gradient-based refinement criteria that specifically target regions with critical behavior. To this end, we extend Novak-Ritter adaptivity [2] by incorporating modified weight functions and dimension dependence. The hyperparameters of the new methods are optimized using Bayesian optimization. We demonstrate the effectiveness of our approach on several test functions, showing promising results. Real-world applications in autonomous driving represent the next step.

- Nidhi Kalra and Susan M. Paddock. "Driving to safety: How many miles of driving would it take to demonstrate autonomous vehicle reliability?" In: *Transportation Research Part A: Policy and Practice* 94 (2016), pp. 182–193. ISSN: 0965-8564. DOI: https://doi.org/10.1016/j.tra.2016. 09.010.
- [2] Erich Novak and Klaus Ritter. "Global Optimization Using Hyperbolic Cross Points". In: State of the Art in Global Optimization: Computational Methods and Applications. Ed. by C. A. Floudas and P. M. Pardalos. Boston, MA: Springer US, 1996, pp. 19–33. ISBN: 978-1-4613-3437-8. DOI: 10.1007/978-1-4613-3437-8_2.
- [3] Julian Valentin and Dirk Pflüger. "Hierarchical Gradient-Based Optimization with B-Splines on Sparse Grids". In: Sparse Grids and Applications - Stuttgart 2014. Ed. by Jochen Garcke and Dirk Pflüger. Cham: Springer International Publishing, 2016, pp. 315–336. ISBN: 978-3-319-28262-6.

Kernel-based approximation of high-dimensional functions with small efficient dimension

Wendland, H.¹

¹Department of Mathematics, University of Bayreuth, 95440 Bayreuth, Germany

Abstract

In this talk, I will discuss the approximation of high-dimensional functions, which are effectively low dimensional. Such functions can be written as the sum of functions depending on fewer variables plus a high-dimensional less significant part.

I will discuss the problem first in a general reproducing kernel Hilbert space set-up and then continue within the specific setting of mixed regularity Sobolev spaces, which often occur in high-dimensional problems. I will show that such problems often do not suffer from the curse of dimensionality. This is achieved by deriving new sampling inequalities and error estimates for specific constructive kernel-based approximation methods.

This talk is based on joint work with Christian Rieger (Marburg University, Germany, [1, 2].

- [1] C. Rieger and H. Wendland. Constructive Approximation of High-Dimensional Functions with Small Efficient Dimension with Applications in Uncertainty Quantification. 2025.
- [2] C. Rieger and H. Wendland. "On the Approximability and Curse of Dimensionality of Certain Classes of High-Dimensional Functions". In: *Siam Journal on Numerical Analysis* 62 (2024), pp. 842–871.

Revisiting the Tensor Product Multilevel Method: New Insights into Kernel-Based Sparse Grid Approximation

Kempf, $R.^1$

¹Applied and Numerical Analysis, University of Bayreuth

Abstract

The *tensor product multilevel method*, introduced in [1], combines the kernel-based multilevel method with the Smolyak algorithm or combination technique. This framework supports arbitrary low-dimensional domains and scattered data, offering a high-order, meshfree strategy for the approximation of functions in high-dimensional settings.

Recent results on the kernel-based multilevel method, in particular a nodal representation of the approximation and subsequent better understanding of the approximation operator's range, enable a sharper theoretical and practical analysis of the tensor product multilevel method and improve on the results obtained in [1].

In this talk, I will first outline the core ideas behind the kernel-based multilevel method and its integration with sparse grid strategies. I will then highlight how the new developments enhance the tensor product multilevel method, both in theory and in computational performance. The presentation will conclude with numerical experiments illustrating the benefits of the improved scheme in moderately to highly dimensional settings.

References

 Rüdiger Kempf and Holger Wendland. "High-dimensional approximation with kernel-based multilevel methods on sparse grids". In: *Numerische Mathematik* 154.3 (2023), pp. 485–519. ISSN: 0029-599X.

Functional Multi-Reference Alignment via Deconvolution

Al-Ghattas, O.¹, Little, A.², Sanz-Alonso, D.¹, and Sweeney, M.²

¹University of Chicago, Department of Statistics ²University of Utah, Department of Mathematics

Abstract

This paper studies the multi-reference alignment problem of estimating a hidden signal function from shifted, noisy observations. By formulating the problem in function space, we uncover a new connection between multi-reference alignment and deconvolution: the signal can be recovered from second order statistics in the Fourier domain by a procedure analogous to Kotlarski's approach to deconvolution. In addition, we extend Kotlarski's identity to general dimension and study the estimation of signals with vanishing Fourier transform, thus filling a gap in the deconvolution literature. We validate our deconvolution approach to multi-reference alignment through both theory and numerical experiments. [1].

References

[1] Omar Al-Ghattas et al. "Functional Multi-Reference Alignment via Deconvolution". In: *arXiv preprint* arXiv:2506.12201 (2025).

Consistent PINNs for parabolic PDEs

Mishra, $S.^1$ and Khan, $A.^2$

¹PhD student, Department of Mathematics, IIT Roorkee, 247667, India (shiv m@ma.iitr.ac.in) ²Associate Professor, Department of Mathematics, IIT Roorkee, 247667, India (arbaz@ma.iitr.ac.in)

Abstract

We present a new a priori analysis of a class of collocation methods for parabolic PDEs specifically for the heat equation with nonhomogeneous Dirichlet boundary conditions that rely only on pointwise data of force term f, boundary data g, and initial data u_0 . Under Besov regularity assumptions, we characterize the optimal recovery rate of the solution u based on sample complexity. We establish error bounds by constructing a new consistent loss function \mathcal{L}^* that effectively controls the approximation error. This loss incorporates contributions from the interior, boundary, and initial data in a discretized form and is designed to reflect the true PDE structure. Our theoretical results show that minimizing \mathcal{L}^* yields near-optimal recovery under suitable regularity and sampling. The novelty of this work lies in characterizing the approximation performance of a function in the space-time domain using Besov model classes and deriving the lower bounds and convergence rates in both interior and boundary norms. Furthermore, we define an error bound for the solution from the proposed consistent loss.

References

[1] S. Mishra and A. Khan. A priori error analysis of consistent PINNs for parabolic PDEs. submitted. 2025.

Path dependent time series models

Teichmann, J.¹

¹ETH Zürich

July 1, 2025

Abstract

We prove a novel stochastic version of Floris Takens famous theorem on delay embeddings from 1981. We apply those insights to constructing path dependent stochastic models for time series modelling in view of financial time series. Path dependence is modelled via randomized signatures, which is a version of signatures capturing features of curves efficiently.

Data-driven identification of port-Hamiltonian DAE systems by Gaussian processes

Zaspel, P.¹ and Günther, M.¹

¹Bergische Universität Wuppertal

Abstract

Port-Hamiltonian systems (pHS) allow for a structure-preserving modeling of dynamical systems. Coupling pHS via linear relations between input and output defines an overall pHS, which is structure preserving. However, in multiphysics applications, some subsystems do not allow for a physical pHS description, as (a) this is not available or (b) too expensive. Here, data-driven approaches can be used to deliver a pHS for such subsystems, which can then be coupled to the other subsystems in a structure-preserving way. In our work [1], we derive a data-driven identification approach for port-Hamiltonian differential algebraic equation (DAE) systems. The approach uses input and state space data to estimate nonlinear effort functions of pH-DAEs. As underlying technique, we us (multi-task) Gaussian processes. This work thereby extends over the current state of the art, in which only port-Hamiltonian ordinary differential equation systems could be identified via Gaussian processes.

References

[1] Peter Zaspel and Michael Günther. Data-driven identification of port-Hamiltonian DAE systems by Gaussian processes. arXiv preprint 2406.18726. 2024.

Adaptive and non-adaptive approximation of high-dimensional vectors

Kunsch, R.¹ and Wnuk, M.²

¹RWTH Aachen University, at the Chair of Mathematics of Information Processing ²Institute of Mathematics, University of Osnabrück

Abstract

We discuss approximation of the embedding $\ell_p^m \hookrightarrow \ell_q^m, 1 \le p < q \le \infty$, based on randomized algorithms that use up to n arbitrary linear functionals as information on a problem instance where $n \ll m$. By analysing adaptive methods we show upper bounds for which the information-based complexity n exhibits only a $(\log \log m)$ -dependence. In the case $q < \infty$ we use a multi-sensitivity approach in order to reach optimal polynomial order in n for the Monte Carlo error. We also improve on non-adaptive methods for $q < \infty$ by denoising known algorithms for uniform approximation. If time permits we also discuss some lower bounds on the performance of randomized algorithms.

Quasi-Monte-Carlo method for Gevrey class functions governed by non-linear PDEs

$L\hat{e}, T.^1$ and Chernov, A.¹

¹Carl von Ossietzky Universität Oldenburg

Abstract

Gevrey class functions play a crucial role in both the analytical and numerical treatment of partial differential equations (PDEs), as they capture a refined notion of smoothness that extends beyond classical analytic regularity. Non-linear PDEs—such as eigenvalue problems [1], semilinear diffusion-reaction equations [2], and the Navier-Stokes equations [3]—are central to modeling complex phenomena in science and engineering, from fluid dynamics to quantitative finance. However, their numerical solution in high dimensions remains challenging due to the well-known "curse of dimensionality".

Quasi-Monte Carlo (QMC) method provide a promising alternative to traditional Monte Carlo techniques by leveraging deterministic sequences with superior distribution properties. This talk present the use of rank-1 lattice rules for efficiently approximating high-dimensional integrals that arise in the solution of non-linear PDEs with Gevrey regularity. A key focus will be on the derivation of error bounds for these lattice rules in the setting of Gevrey-class functions, offering rigorous theoretical justification for accuracy and efficiency of QMC method. These result naturally extends [4] and contributes to the development of robust numerical methods for tackling high-dimensional, non-linear problems across a range of applications.

- A. Chernov and T. Lê. "Analytic and gevrey class regularity for parametric elliptic eigenvalue problems and applications". In: SIAM Journal on Numerical Analysis 62 (2024), pp. 1874–1900.
- [2] A. Chernov and T. Lê. "Analytic and gevrey class regularity for parametric semilinear reactiondiffusion problems and applications in uncertainty quantification". In: Computers & Mathematics with Applications 164 (2024), pp. 116–130.
- [3] A. Chernov and T. Lê. Gevrey class regularity for steady-state incompressible Navier-Stokes equations in parametric domains and related models. preprint, aRxiv:2504.13753. 2025.
- [4] F. Y. Kuo, C. Schwab, and I. H. Sloan. "Quasi-monte carlo finite element methods for a class of elliptic partial differential equations with random coefficients". In: SIAM Journal on Numerical Analysis 50 (2012), pp. 3351–3374.

A framework for proving parametric regularity of high-dimensional problems

Harbrecht, H.¹, Schmidlin, M.¹, and Schwab, Ch.²

¹Universität Basel, Departement Mathematik und Informatik. ²ETH Zürich, Seminar für Angewandte Mathematik.

Abstract

It is well-known that, to be able to approximate high-dimensional problems, it is necessary to exploit as much structure (e.g. symmetry or regularity) of the problem as possible, so as to be able to mitigate the curse of dimensionality. Therefore, we will present a modular and abstract approach for proving parametric regularity of high-dimensional problems that are for example encountered in the context of uncertainty quantification for PDEs or approximating the data-to-solution map of a parametric PDE. This framework is based on quantitative regularity results of Gevrey class-type concerning both the composition of maps and implicitely defined maps between Banach spaces and enables one to study the regularity of high-dimensional problems that fulfil a nonlinear operator equation defined in Banach spaces. We will demonstrate how these mathematical tools can be used to verify the analytic and Gevrey smooth dependence of the solution of a semilinear elliptic PDE on data such as for example the diffusion coefficient or a domain mapping, both as an element of a suitable function space or when given by some (possibly nonlinear) parametric expansion. Moreover, we will comment on how the approach may be used for other nonlinear PDEs. The talk is mainly based on the results contained in [1] and [2].

- H. Harbrecht, M. Schmidlin, and C. Schwab. "The Gevrey class implicit mapping theorem with application to UQ of semilinear elliptic PDEs". In: *Mathematical Models and Methods in Applied Sciences* 34.05 (2024), pp. 881–917.
- M. Schmidlin. "Regularity analysis for semilinear elliptic PDEs with random data". PhD thesis. Basel Switzerland: Universität Basel, Mar. 2024.

Domain UQ for stationary and time-dependent PDEs using QMC

Djurdjevac, A.¹, Kaarnioja, V.¹, Schillings, C.¹, and Zepernick, A.-A.¹

¹Freie Universität Berlin

Abstract

The problem of modelling processes with partial differential equations posed on random domains arises in various applications like biology or engineering. We study uncertainty quantification for partial differential equations subject to domain uncertainty. For the random domain parameterization, we adopt an approach, which was also examined by Chernov and Lê [1, 2] as well as Harbrecht, Schmidlin, and Schwab [4], where one assumes the input random field to be Gevrey regular. This approach has the advantage of being substantially more general than models which assume a particular parametric representation of the input random field such as a Karhunen–Loève series expansion. As model problems we consider both the Poisson equation as well as the heat equation and design randomly shifted lattice quasi-Monte Carlo (QMC) cubature rules for the computation of response statistics subject to domain uncertainty. The QMC rules obtained in [3] exhibit dimension-independent, fasterthan-Monte Carlo cubature convergence rates. Our theoretical results are illustrated by numerical examples.

- [1] A. Chernov and T. Lê. Analytic and Gevrey class regularity for parametric elliptic eigenvalue problems and applications. 2024.
- [2] A. Chernov and T. Lê. Analytic and Gevrey class regularity for parametric semilinear reactiondiffusion problems and applications in uncertainty quantification. 2024.
- [3] A. Djurdjevac et al. Uncertainty quantification for stationary and time-dependent PDEs subject to Gevrey regular random domain deformations. (Preprint). 2025.
- [4] H. Harbrecht, M. Schmidlin, and C. Schwab. The Gevrey class implicit mapping theorem with application to UQ of semilinear elliptic PDEs. 2024.

Quasi-uniform quasi-Monte Carlo point sets and sequences

Goda, $T.^1$

¹Graduate School of Engineering, The University of Tokyo

Abstract

We study the quasi-uniformity properties of quasi-Monte Carlo (QMC) point sets and sequences, with a particular focus on two major classes: digital nets and sequences, and lattice-based constructions.

For digital nets and sequences, we introduce the concept of *well-separated* point sets and provide an algebraic criterion to determine whether a given digital net is quasi-uniform. This condition leads to an explicit construction of a two-dimensional digital net that is both quasi-uniform and lowdiscrepancy. On the other hand, we also provide several counterexamples that are low-discrepancy but not quasi-uniform.

For lattice point sets and sequences, tools from the geometry of numbers allow us to find a sufficient condition under which a lattice in \mathbb{R}^d yields a quasi-uniform point set. This condition is then used to construct explicit two-dimensional examples of quasi-uniform, low-discrepancy lattices. In higher dimensions, we prove the existence of quasi-uniform, low-discrepancy rank-1 lattice point sets.

This talk is based on joint works with Josef Dick, Gerhard Larcher, Friedrich Pillichshammer, and Kosuke Suzuki.

(Near-)Optimality of Quasi–Monte Carlo methods and Suboptimality of the Sparse-Grid Gauss–Hermite Rule in Gaussian Sobolev Spaces

Goda, T¹, Kazashi, Y², and Suzuki, Y³

¹University of Tokyo, Japan ²University of Manchester, UK ³Aalto University, Finland

Abstract

Numerical integration with respect to the standard Gaussian measure is fundamental in many disciplines. Often, target functions belong to the L^2 -Sobolev space of dominating mixed-smoothness, where integrability is with respect to the standard Gaussian measure. In one dimension, the trapezoidal rule is asymptotically optimal in terms of the number of function evaluations in the sense of worst-case error in this space, up to a logarithmic factor that may not be sharp, as shown in [1]. By contrast, Gauss-Hermite quadrature converges at only half this rate. A similar pattern holds for analytic functions. We show that these results extend to higher dimensions: several quasi-Monte Carlo methods achieve the optimal rate (again, up to a logarithmic factor) in this Sobolev space, whereas the Smolyak-type sparse grid based on Gauss-Hermite quadrature attains only half the optimal rate.

References

[1] Yoshihito Kazashi, Yuya Suzuki, and Takashi Goda. "Suboptimality of Gauss-Hermite quadrature and optimality of the trapezoidal rule for functions with finite smoothness". In: *SIAM J. Numer. Anal.* 61.3 (June 30, 2023), pp. 1426–1448. ISSN: 0036-1429, 1095-7170. DOI: 10.1137/22M1480276.

Data Compression using Rank-1 Lattices for Parameter Estimation in Machine Learning

Gnewuch, M.¹, Harsha, K.¹, and Wnuk, M.¹

¹University of Osnabrück

Abstract

The mean squared error and regularized versions of it are standard loss functions in supervised machine learning. However, calculating these losses for large data sets can be computationally demanding. Modifying an approach of J. Dick and M. Feischl [1] we present algorithms to reduce extensive data sets to a smaller size using rank-1 lattices. Rank-1 lattices are quasi-Monte Carlo (QMC) point sets that are, if carefully chosen, well-distributed in a multi-dimensional unit cube. The compression strategy in the preprocessing step assigns every lattice point a pair of weights depending on the original data and responses, representing its relative importance. As a result, the compressed data makes iterative loss calculations in optimization steps much faster. We analyze the errors of our QMC data compression algorithms and the cost of the preprocessing step for functions whose Fourier coefficients decay sufficiently fast so that they lie in certain Wiener algebras or Korobov spaces. In particular, we prove that our approach can lead to arbitrary high convergence rates as long as the functions are sufficiently smooth. The talk is mainly based on the preprint [2].

- [1] Josef Dick and Michael Feischl. "A quasi-Monte Carlo data compression algorithm for machine learning". In: *Journal of Complexity* 67 (2021), p. 101587.
- [2] Michael Gnewuch, Kumar Harsha, and Marcin Wnuk. Data compression using rank-1 lattices for parameter estimation in machine learning. Preprint, arXiv:2409.13453. 2024.

Minimal Subsampled Rank-1 Lattices for Multivariate Approximation with Optimal Convergence Rate

Bartel, F.¹, Gilbert, A. D.¹, Kuo, F. Y.¹, and Sloan, I. H.¹

$^1\mathrm{School}$ of Mathematics and Statistics, University of New South Wales, Sydney NSW 2052, Australia

Abstract

In this talk we show error bounds for randomly subsampled rank-1 lattices. We pay particular attention to the ratio of the size of the subset to the size of the initial lattice, which is decisive for the computational complexity. In the special case of Korobov spaces, we achieve the optimal polynomial sampling complexity whilst having the smallest initial lattice possible. We further characterize the frequency index set for which a given lattice is reconstructing by using the reciprocal of the worst-case error achieved using the lattice in question. This connects existing approaches used in proving error bounds for lattices. We make detailed comments on the implementation and test different algorithms using the subsampled lattice in numerical experiments.

A novel CBC construction for lattice rules for L^2 approximation with POD and SPOD weights

Gilbert, A. D.¹ and Sloan, I. H.¹

¹UNSW Sydney, Sydney NSW 2052 Australia

Abstract

Along with their great success at computing high-dimensional integrals, (rank 1) lattice rules are also useful for approximating periodic functions. For example, lattice rules can be used for kernel interpolation or to approximate the Fourier series of the function in question, where in both cases the lattice structure can be exploited to compute the approximation in a "fast" way. In this talk, we introduce a novel component-by-component (CBC) construction for lattice rules to be used for L^2 approximation of periodic functions belonging to a Korobov space of smoothness $\alpha > \frac{1}{2}$ with either POD (product and order dependent) or SPOD (smoothness-driven product and order dependent) weights. As in the exisiting CBC construction for approximation from Cools, Kuo, Nuvens & Sloan [1], our algorithm aims to sequentially minimise a surrogate for the worst-case error in each dimension. However, our algorithm is simpler to implement and removes the need to look ahead and account for future weights. This means that our construction is extensible in dimension and also cheaper to implement in terms of the dependence of the cost on the dimension. Our construction can also be done in a fast way using the usual tricks with the fast Fourier transform. We will present numerical results where our surrogate for the worst-case error behaves empirically very similarly to the existing CBC from [1]. We also prove that the resulting worst-case error for an N-point lattice rule satisfies a bound with the same rate $O(N^{-\alpha/2+\epsilon})$, for $\epsilon > 0$ and smoothness $\alpha > \frac{1}{2}$, although our constant is larger than in the previous bound.

References

[1] R. Cools et al. "Fast component-by-component algorithms for lattice algorithms for multivariate approximation with POD and SPOD weights". In: *Math. Comp.* 90 (2022), pp. 717–812.

The Quality of Lattice and Kronecker Sequences

Hickernell, F. J.¹, Hall, Jr., C.¹, and Matiukha, L.¹

¹Illinois Institute of Technology, Chicago, IL, USA

July 1, 2025

Abstract

Two families of low discrepancy sequences defined on the half-open unit cube, $[0,1)^d$, are shifted lattice sequences, $\{\phi_b(i)\mathbf{h} + \mathbf{\Delta} \mod \mathbf{1}\}_{i=0}^{\infty}$ [1], and shifted Kronecker sequences, $\{i\mathbf{\alpha} + \mathbf{\Delta} \mod \mathbf{1}\}_{i=0}^{\infty}$. Here,

- $\{\phi_b(i)\}_{i=0}^{\infty}$ is the van der Corput sequence in prime base b,
- h is a generalized (infinite number of digits) d-dimensional, positive integer vector, which generates the lattice sequence,
- $\boldsymbol{\alpha} \in [0,1)^d$ generates the Kronecker sequence, and
- $\Delta \in [0,1)^d$ is a (random) shift.

Multidimensional integrals may be approximated by the sample means of function values:

$$\int_{[0,1)^d} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \approx \frac{1}{n} \sum_{i=0}^{n-1} f(\boldsymbol{x}_i).$$

For lattice sequences, choosing the first $n = b^m$ points for non-negative integer m preserves the lattice structure and generally gives a better approximation than arbitrary n. For Kronecker sequences, there is no preferred sample size, and the choice of the generating vector has been less studied relatively.

This talk describes the performance of these two low discrepancy families for cubature for arbitrary n. We also explore cubatures of the form $\sum_{i=0}^{n-1} w_i f(\boldsymbol{x}_i)$ with nonconstant sample weights $\{w_i\}_{i=0}^{n-1}$. We compare lattice and Kronecker sequences to other low discrepancy points by way of figures of merit and performance on test cases.

References

 J. Dick, P. Kritzer, and F. Pillichshammer. Lattice Rules: Numerical Integration, Approximation, and Discrepancy. Springer Series in Computational Mathematics. Springer Cham, 2022. DOI: https: //doi.org/10.1007/978-3-031-09951-9.

Dimension-independent convergence rates of median randomized nets

Pan, Z^1

¹RICAM, Austrian Academy of Sciences

Abstract

Recent advances in quasi-Monte Carlo integration demonstrate that the median of linearly scrambled digital net estimators achieves near-optimal convergence rates for high-dimensional integrals without requiring a priori knowledge of the integrand's smoothness [2]. Building on this framework, we prove that the median estimator attains dimension-independent convergence under tractability conditions characterized by low effective dimensionality, a property known as strong tractability in complexity theory [1]. Our analysis strengthens existing guarantees by improving the convergence rates and relaxing the theoretical assumptions previously required for strong tractability.

- [1] E. Novak and H. Wozniakowski. Tractability of multivariate problems. 2008.
- [2] Z. Pan. Automatic optimal-rate convergence of randomized nets using median-of-means. 2025.
- [3] Z. Pan. Dimension-independent convergence rates of randomized nets using median-of-means. 2025.

Median lattice rules for function approximation

Goda, T.², Kritzer, P.¹, and Pan, Z.¹

¹Austrian Academy of Sciences ²The University of Tokyo

Abstract

We consider L_2 -approximation of functions in a weighted Korobov space. We present a median algorithm, which is related to median integration rules, that have recently gained a lot of interest in the theory of quasi-Monte Carlo methods. Indeed, we use lattice rules as the underlying integration rules to approximate Fourier coefficients. As we will show, we can obtain a convergence rate that is arbitrarily close to optimal in terms of the number of evaluations needed of the function to be approximated.

Least squares using Kronecker points

Nuyens, D.¹, Cools, R.¹, and Wilkes, L.¹

¹KU Leuven, Belgium

Abstract

We analyse the least squares method for approximating multivariate periodic functions using n function values. The point sets are so-called "Kronecker point sets" or "generated sets" [3]. A Kronecker point set with n points is defined by a generator $\boldsymbol{\zeta} \in \mathbb{R}^d$ and the points are then given by

 $\boldsymbol{x}_k = \boldsymbol{\zeta} k \mod 1$ for $k = 1, \dots, n$.

We prove existence of a generator $\boldsymbol{\zeta}$ with the almost optimal L_2 error convergence. We also prove a modification for rational generators, in which case our method is similar to subsampled rank-1 lattices [1], except that we just take the initial points and do not need to subsample. Our bounds are slightly worse than those obtained in [4] for the periodic setting, but [4] uses unstructured points. The results can be found in the preprint [2].

- F. Bartel et al. "On the reconstruction of functions from values at subsampled quadrature points". In: Mathematics of Computation 93 (2024), pp. 785–809.
- R. Cools, D. Nuyens, and L. Wilkes. "Error bounds for function approximation using generated sets". https://arxiv.org/abs/2505.00440. 2025.
- [3] L. Kämmerer. "Reconstructing multivariate trigonometric polynomials by sampling along generated sets". In: Monte Carlo and Quasi-Monte Carlo Methods 2012. Ed. by J. Dick et al. Springer-Verlag, 2013, pp. 439–454.
- [4] D. Krieg and M. Ullrich. "Function values are enough for L₂ approximation". In: Foundations of Computational Mathematics 21 (2021), pp. 1141–1151.

Minimization of Costly Functions Using Sparse FFT-Based Interpolation

Zhou, Y.¹, Naert, K.², Nuyens, D.¹, and Weiwen, M.¹

 $^1 \rm Department$ of Computer Science, KU Leuven, Belgium $^2 \rm Digital$ Solutions & Innovation, Arcelor
Mittal Belgium, Belgium

Abstract

It is challenging to minimize a costly function with limited samples. We propose a method that interpolates such functions from samples at rank-1 lattice points. This significantly reduces the computational cost typically associated with dense sampling. Preliminary results demonstrate the method's effectiveness for smooth, periodic functions.

Near-Optimal Learning of Lipschitz Operators with respect to Gaussian Measures

Adcock, B.¹, Griebel, M.^{2,3}, and Maier, G.^{2,3}

¹Simon Fraser University ²University of Bonn ³Fraunhofer Institute for Algorithms and Scientific Computing (SCAI)

Abstract

Operator learning, the approximation of mappings between infinite-dimensional function spaces using machine learning, has gained increasing research attention in recent years. Approximate operators, learned from data, hold promise to serve as efficient surrogate models for problems in computational science and engineering, complementing traditional numerical methods. Despite their empirical success, our understanding of the underpinning mathematical theory is in large part still incomplete. Previous research efforts mainly focused on the analysis of holomorphic and linear operators. However, far less is known about the learnability of nonlinear operators that are merely Lipschitz continuous, which arise, for example, as parameter-to-solution mappings in parametric variational inequalities.

In this talk, we study the approximation of Lipschitz operators in expectation with respect to Gaussian measures. We consider general reconstruction strategies from m arbitrary (potentially adaptive) linear samples and tightly characterize the corresponding sample complexity, that is, the smallest achievable worst-case error among all possible choices of (adaptive) linear sampling and arbitrary reconstruction methods, in terms of m. As a result, we identify an inherent curse of sample complexity: No method (polynomials, neural networks, kernel methods, etc.) to approximate Lipschitz operators on infinite-dimensional domains based on m linear samples can achieve algebraic convergence rates in m (see [1] for further details). This result is complemented with an analysis of the sample complexity of learning Lipschitz operators on finite-dimensional domains. In this setting, we prove optimal rates which are algebraic in m but subject to the classical curse of dimensionality. Finally, we combine our findings to propose a data-driven algorithm for the recovery of Lipschitz operators from finitely many noisy data samples which provably achieves near-optimal sample complexity.

References

[1] Ben Adcock, Michael Griebel, and Gregor Maier. Learning Lipschitz Operators with respect to Gaussian Measures with Near-Optimal Sample Complexity. arXiv:2410.23440. 2025.

On Sobolev and Besov Spaces With Hybrid Regularity

Harbrecht, H.¹ and von Rickenbach, R.¹

 1 Universität Basel

Abstract

This talk is concerned with the nonlinear approximation of functions in the Sobolev space H^q using a tensor-product, or hyperbolic wavelet basis on the unit *n*-cube. Here, *q* is a real number, which is not necessarily positive. We derive Jackson and Bernstein inequalities to obtain that the approximation classes contain Besov spaces of hybrid regularity in the sense of [1, 3]. Moreover, we are going to compare these resulting approximation classes with those corresponding to isotropic wavelet bases following [2]. Especially, we show that the classical Besov spaces $B_{\tau}^{q+sn,\tau}$, where $\frac{1}{\tau} = s + \frac{1}{2}$, are included in the Besov spaces of hybrid regularity $\mathfrak{B}_{\tau}^{q,s,\tau}$. Herein, *q* denotes the isotropic regularity and *s* the additional mixed regularity. In particular, this implies that all functions which can be approximated by classical wavelets are also approximable by tensor-product wavelets at least at the same rate.

- Glenn Byrenheid, Janina Hübner, and Markus Weimar. "Rate-optimal sparse approximation of compact break-of-scale embeddings". In: Applied and Computational Harmonic Analysis 65 (2023), pp. 40–66.
- Helmut Harbrecht and Remo von Rickenbach. On Sobolev and Besov Spaces with Hybrid Regularity. Preprint, arXiv:2411.04837. 2024.
- [3] Pál-Andrej Nitsche. "Best N Term Approximation Spaces for Tensor Product Wavelet Bases". In: Constructive Approximation 24.1 (2006), pp. 49–70.

Uncertainty quantification of spectral clusterings

Dölz, J.¹ and Weygandt, J.¹

¹University of Bonn

Abstract

Spectral clustering is a popular unsupervised learning technique which is able to partition unlabelled data into disjoint clusters of distinct shapes. However, the data under consideration are often experimental data, implying that the data is subject to measurement errors and measurements may even be lost or invalid. These uncertainties in the corrupted input data induce corresponding uncertainties in the resulting clusters, and the clusterings thus become unreliable.

Modelling the uncertainties as random processes, we discuss a mathematical framework based on random set theory for the computational Monte Carlo approximation of statistically expected clusterings in case of corrupted, i.e., perturbed, incomplete, and possibly even additional, data. We propose several computationally accessible quantities of interest and analyze their consistency in the infinite data point and infinite Monte Carlo sample limit. Numerical experiments are provided to illustrate and compare the proposed quantities.

References

[1] Jürgen Dölz and Jolanda Weygandt. Quantifying uncertainty in spectral clusterings: expectations for perturbed and incomplete data. 2025.

Approximations of Differential Entropy in Bayesian Optimal Experimental Design

Chen, C.¹, Helin, T.¹, Hyvönen, N.², and Suzuki, Y.²

¹LUT University ²Aalto University

Abstract

We present a method to approximate differential entropy, which is then used to maximize the expected information gain, commonly used in Bayesian Optimal Experimental Design (BOED). We consider the standard additive noise model

$$y = \mathcal{G}(x;\xi) + \varepsilon,$$

where $y \in \mathbb{R}^d$ is the observed data, \mathcal{G} denotes the forward map, $x \in \mathcal{X}$ is the quantity of interest, ξ is the design variable, and ε is the additive noise. We assume that ε is Gaussian and does not depend on the design ξ . We want to maximize expected information gain,

$$\begin{split} U(\xi) &:= \iint_{\mathbb{R}^d \times \mathcal{X}} \left[\log \frac{\pi(y|x;\xi)}{\pi(y;\xi)} \right] \pi(x,y;\xi) \mathrm{d}x \mathrm{d}y \\ &= - \int_{\mathbb{R}^d} \log \left(\pi\left(y;\xi\right) \right) \pi(y;\xi) \mathrm{d}y + \iint_{\mathbb{R}^d \times \mathcal{X}} \left(\pi\left(y|x;\xi\right) \right) \pi(y|x;\xi) \mathrm{d}y \mu(x) \mathrm{d}x \end{split}$$

where $\pi(x, y; \xi)$ stands for the joint distribution, $\pi(y|x; \xi)$ is the likelihood, $\pi(y; \xi)$ is the evidence, and $\mu(x)$ is the prior. In this setting, the second term above is independent of ξ . Thus we only need to maximize the first term, the differential entropy of the evidence.

We assume that evaluation of the forward map \mathcal{G} is the dominant cost of the problem, and we want to reduce the number of forward map evaluations, say M, as much as possible. To this end, we construct a surrogate model of the evidence $\pi(y;\xi)$. We show that our proposed method can attain the convergence rate $\mathcal{O}(M^{-1/2})$, and this can be accelerated by quasi-Monte Carlo methods. We also numerically demonstrate our method for a PDE problem where the dimensionality of \mathcal{X} is high.

Discontinuous Galerkin discretization of conservative dynamical low-rank approximation schemes for the Vlasov–Poisson equation

Zeiser, A¹ and Uschmajew, A²

¹Faculty 1: School of Engineering – Energy and Information, HTW Berlin – University of Applied Sciences, 12459 Berlin, Germany

²Institute of Mathematics & Centre for Advanced Analytics and Predictive Sciences, University of Augsburg, 86159 Augsburg, Germany

Abstract

We present a novel numerical scheme for the Vlasov-Poisson equation based on dynamical low-rank approximation (DLRA) [1]. Our method combines a continuous formulation of the DLRA evolution equations as Friedrichs' systems with a discontinuous Galerkin (DG) discretization in space and rank-adaptive time integration. We show that our method preserves mass and momentum at the discrete level.

To demonstrate the robustness and accuracy of the proposed method, we present numerical experiments in one and two spatial dimensions for the benchmark problem of Landau damping. Furthermore, we illustrate the feasibility of combining our low-rank solver with mesh adaptivity within the DG framework, leading to a fully adaptive method that is both efficient and accurate.

This work contributes to the growing body of research on low-rank methods for kinetic equations, opening new directions for the development of high-performance solvers.

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Dimensionality reduction techniques for numerical solutions of the Elder problem

Khotyachuk, R.¹ and Johannsen, K.²

¹University of Bergen ²NORCE Norwegian Research Center AS

Abstract

Keywords: The Elder problem, dimensionality reduction, feature engineering, data complexity

In this work, we considered applying Machine Learning (ML) methods to the analysis of numerical solutions of partial differential equations (PDEs). In particular, we have applied some dimensionality reduction (DR) techniques to numerical solutions of the Elder problem (EP) [6].

We performed large-scale simulations and obtained large ensembles of perturbed solutions of the EP [7]. Based on these high-fidelity datasets, we have evaluated various approaches to DR, including feature selection and feature extraction, aimed at building ML models for predicting steady states of the EP using classification algorithms [4].

We considered the following DR techniques in this work:

- Univariate feature selection based on different filter functions [3, 5].
- Linear methods [2]: LDA, PCA, NMF, Sx-Basis projection.
- Nonlinear methods (Manifold Learning) [9]: KernelPCA, ISOMAP, LLE, LEM.
- Autoencoders(AE) [1]: fully-connected AE, convolutional AE.

The performance comparison for the abovementioned DR techniques was conducted based on the following measures:

- 1. Reconstruction error when reconstructing the original high-dimensional dataset from a low-dimensional embedding.
- 2. Classification accuracy of predictive models based on features obtained using different DR methods.
- 3. Data complexity metrics [8] for the original and reduced datasets.

Uncertainty estimations were performed for all results of this study using the Bootstrap resampling.

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Higher Order Singularities in High Dimensions

Flad, H.-J.¹

¹Institut für Numerische Simulation, Universität Bonn, Friedrich-Hirzebruch-Allee 7, 53115 Bonn

Abstract

Configuration spaces of many-particle systems represent a generic class of high dimensional problems where various types of singularities appear at coalescence points of particles. These singularities can be classified into conic, edge and higher order corner singularities depending on the number of particles at the coalescence points. It goes without saying that these singularities have a severe impact concerning regularity issues and approximation properties of functions on these spaces.

We present an analytic approach to higher order singularities in configurations space [1] which enables a canocial completion in the geometric sense such that singularities of various order intersect transversally. This completion agrees with the Fulton-MacPherson compactification of configuration space in algebraic geometry [2] which has already found various applications in physics. The functional analytic setting including stratification, function spaces and a recursive parametrix (pseudoinverse) construction for elliptic operators will be briefly discussed. Finally, we mention possible implications for modelling, approximation and numerical analysis on configuration spaces.

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Sampling recovery in Bochner spaces and applications to parametric PDEs with random inputs

Dinh, $D.^1$

¹Information Technology Institute, Vietnam National University 144 Xuan Thuy, Cau Giay, Hanoi, Vietnam Email: dinhzung@gmail.com

Abstract

We proved convergence rates of linear sampling recovery of functions in an abstract Bochner space satisfying some weighted summability of their generalized polynomial chaos expansion coefficients, which are realized by extended least squares methods to this space. As applications to a problem in Computational Uncertainty Quantification, we derived convergence rates of linear collocation approximation of solutions to parametric elliptic or parabolic PDEs with log-normal random inputs, and of relevant infinite-dimensional holomorphic functions. These convergence rates significantly improve the known results. From the general results we also received the same convergence rates of linear collocation approximation of solutions to parametric PDEs with affine random inputs.

This talk is based on the joint work [1].

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Optimal solvers for infinite-dimensional sparse approximations in adaptive stochastic Galerkin finite element methods

Eisenmann, H.¹, Bachmayr, M.¹, Eigel, M.², and Voulis, I.³

¹RWTH Aachen ²WIAS Berlin ³Universität Göttingen

Abstract

For a class of elliptic diffusion problems on a domain D, we aim to approximate the mapping from diffusion coefficients a = a(y) to the corresponding solutions u. We treat here the case of infinitely many parameters, which is common when random fields are represented in series expansions. We show convergence with uniform rate of an adaptive stochastic Galerkin method, and given an expansion of the random field of the form

$$a(y) = f\left(\sum_{j \in \mathbb{N}} \sum_{k \in \mathbb{N}} y_{j,k} \theta_{j,k}(x)\right)$$

with functions $\theta_{j,k}$ having multilevel structure, and an analytic function f, it is shown to produce quasi-optimal approximations with almost optimal computational costs.

The solution map is well approximated by a series

$$\tilde{u}(x,y) = \sum_{\nu \in F} u_{\nu}(x) L_{\nu}(y)$$

with function valued coefficients u_{ν} and product Legendre polynomials L_{ν} . For this expansion to have a quasi-optimal number of degrees of freedom, it is essential to allow each function u_{ν} to be approximated in a different discrete space $V_{\nu} \subset H_0^1(D)$.

We utilize finite element frames when estimating the residual to circumvent problems arising jump discontinuities of the residual on an overlay of many different meshes. This allows to show the saturation property, that is, error reduction by a uniform factor in each step. For optimality, we show a stability property of finite element subframes connected to conforming triangulations.

DICE: Discrete inverse continuity equation for learning population dynamics

Blickhan, T.¹, Berman, J.¹, Stuart, A.², and Peherstorfer, B.¹

¹Courant Institute of Mathematical Sciences, New York University ²Computing and Mathematical Sciences, California Institute of Technology

Abstract

We introduce the Discrete Inverse Continuity Equation (DICE) method, a generative modeling approach that learns the evolution of a stochastic process from given sample populations at a finite number of time points. Models learned with DICE capture the typically smooth and well-behaved population dynamics, rather than the dynamics of individual sample trajectories that can exhibit complex or even chaotic behavior. The DICE loss function is developed specifically to be invariant, even in discrete time, to spatially constant but time-varying spurious constants that can emerge during training; this invariance increases training stability and robustness. Generating a trajectory of sample populations with DICE is fast because samples evolve directly in the time interval over which the stochastic process is formulated, in contrast to approaches that condition on time and then require multiple sampling steps per time step. DICE is stable to train, in situations where other methods for learning population dynamics fail, and DICE generates representative samples with orders of magnitude lower costs than methods that have to condition on time. Numerical experiments on a wide range of problems from random waves, Vlasov-Poisson instabilities and high-dimensional chaos are included to justify these assertions.

References

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Sparse and low-rank approximations of parametric PDEs: the best of both worlds

Bachmayr, M.¹ and Yang, H.¹

¹Institut für Geometrie und Praktische Mathematik, RWTH Aachen University

Abstract

We introduce a new type of sparse and low-rank approximation for solutions of parametric partial differential equations depending on infinitely many parameters, combining low-rank tensor approximation in a subset of dominant parameters with a sparse polynomial expansion in the remaining variables. This differs from usual low-rank approaches for such problems based on separating all variables, and it addresses in particular classes of elliptic problems - for example, with random diffusion coefficients of short correlation length - where a direct polynomial expansion is inefficient.

Based on this approximation format, we propose a convergent adaptive Galerkin solver that uses tensor soft thresholding for rank reduction and refines discretizations based on lower-dimensional projected quantities. Unlike existing adaptive low-rank schemes, we obtain quasi-optimal ranks of all iterates and at the same time optimal convergence rates of spatial discretizations without a coarsening step. The results are illustrated by numerical tests.

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