Plenary Talks

Mon, July 28 14:00–15:00

Golden ratio nets and sequences

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In this talk, we discuss nets and sequences constructed in an irrational base, focusing on the case of a base given by the golden ratio φ. We provide a complete framework to study equidistribution properties of nets in base φ, which among other things requires the introduction of a new concept of prime elementary intervals which differ from the standard definition used for integer bases. We define the one-dimensional van der Corput sequence in base φ and two-dimensional Hammersley point sets in base φ and we prove some properties for $(0,1)-$sequences and $(0,m,2)-$nets in base φ, respectively. This part of the talk is based on [1].

Building on this new framework, we propose an *interlaced Halton sequence* that makes use of integer *and* irrational-based van der Corput sequences and show empirically improved performance compared to the traditional Halton sequence [2]. In addition, we propose a scrambling algorithm for irrational-based digital sequences, which leverages dependence properties of scrambled digital nets [3].

[1] N. Kirk, C. Lemieux and J. Wiart. Golden ratio nets and sequences. To appear in *Functiones and Approximatio*, 2025.

[2] N. Kirk, C. Lemieux. An improved Halton sequence for implementation in quasi-Monte Carlo methods. *Proceedings of the 2024 Winter Simulation Conference*, 431–442, IEEE Press, Piscataway, NJ, 2024.

[3] C. Lemieux and J. Wiart. On the distribution of scrambled $(0,m,s)$-nets over unanchored boxes. In: *Monte Carlo and Quasi-Monte Carlo Methods 2020*, A. Keller (ed), Springer, 187-230, 2022.

Tue, July 29 09:00–10:00

Combining Simulation and Linear Algebra: COSIMLA

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In numerical computation for Markov chains and jump processes, matrix-based linear algebraic methods leverage fully the special structure of such models, allowing one to efficiently compute highly accurate solutions quickly. When the number of states is large or infinite, Monte Carlo simulation is an appealing alternative, typically allowing low accuracy solutions to be computed efficiently. In this talk, we describe COSIMLA, COmbined SIMulations and Linear Algebra. This new class of algorithms combines the best of the two numerical approaches, using matrix methods to compute expectations and probabilities in the truncated core of the state space, while one uses Monte Carlo to simulate path excursions outside the truncation. As a result, one can now compute high accuracy solutions for models with a very large state space. We show how the method applies to computing equilibrium quantities and various transient characteristics of Markov chains. These algorithms can typically be viewed as an application of conditional Monte Carlo. We also discuss how stratification can be conveniently applied in this setting to provide further variance reductions.

Tue, July 29 14:00–15:00

Sensitivity and Screening: From Monte Carlo to Experimental Design

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Identifying the most important factors affecting the output of a system from a set of potentially important factors is an important problem in scientific investigations. If a computational model is available to predict the output, we can use global sensitivity analysis to quantify the importance of each factor. There are many Monte Carlo-based methods available to estimate global sensitivity indices. However, their computation can become costly if the model is computationally expensive. In such cases, carefully designed experiments can be used for screening the factors. In this talk, I will explain some of these techniques and the latest developments, including their applications in active learning. I will also briefly explain how to estimate the sensitivity indices from noisy data when we do not know or have access to the model that generated the data.

[1] Xiao, Q., Joseph, V. R., and Ray, D. M. (2023). *Maximum One-Factor-At-A-Time Designs for Screening in Computer Experiments*. Technometrics, 65, 220-230.

[2] Song, D. and Joseph, V. R. (2025). *Efficient Active Learning Strategies for Computer Experiments*. https://arxiv.org/abs/2501.13841.

[3] Huang, C. and Joseph, V. R. (2025). *Factor Importance Ranking and Selection using Total Indices*. Technometrics, https://doi.org/10.1080/00401706.2025.2483531.

Wed, July 30 09:00–10:00

An optimal transport approach to quantifying model uncertainty of SDEs

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A fundamental question in stochastic modelling is that of quantifying the effects of model uncertainty. In this context it is of interest to compute a distance between different stochastic models. A reasonable choice of distance is a modification of the Wasserstein distance on the space of probability measures called adapted Wasserstein distance, as it appears in bicausal optimal transport.

We solve constrained optimal transport problems in which the marginal laws are given by the laws of solutions of stochastic differential equations (SDEs). We consider SDEs with irregular coefficients, making only minimal regularity assumptions. Numerical methods are employed as a theoretical tool to bound the adapted Wasserstein distance. This opens the door for computing the adapted Wasserstein distance in a simple way. We show that this method can be applied to quantifying model uncertainty in stochastic optimisation problems.

Our approach successfully brings together optimal transport and numerical analysis of SDEs.

Thu, July 31 09:00–10:00

Gradient-Based MCMC Sampling: Methods and Optimization Strategies

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Gradient-based Markov Chain Monte Carlo (MCMC) methods significantly outperform gradient-free alternatives in sampling efficiency, particularly in high-dimensional spaces where they have become the standard approach. These methods leverage gradient information to guide the sampling process more intelligently than random-walk approaches. Two fundamental approaches that dominate this field are 1) Hamiltonian Monte Carlo (HMC), which employs principles from classical mechanics, treating the sampling problem as simulating Hamiltonian dynamics on an extended phase space. This approach naturally incorporates momentum variables that help the sampler traverse the parameter space more efficiently than simple random walks. 2) Langevin Monte Carlo (LMC), which utilizes stochastic differential equations that incorporate both gradient information and controlled noise injection. Recent theoretical developments have produced microcanonical versions of both Hamiltonian and Langevin samplers (MCHMC and MCLMC). These variants demonstrate measurably superior sampling efficiency compared to their canonical predecessors.

In addition to the choice of the method, practitioners face numerous algorithmic choices that can significantly impact performance: 1) Metropolis Adjustment: The decision whether to include Metropolis-Hastings correction steps involves trading exact preservation of the target distribution against computational speed. 2) Preconditioning: Incorporating problem-specific geometric information through preconditioning matrices can dramatically improve convergence rates, particularly for ill-conditioned target distributions. 3) Hyperparameter Tuning: Critical parameters include step sizes, trajectory lengths for HMC, and damping coefficients for Langevin methods. Recently, well tuned black-box methods have been developed that approach optimal performance. 4) Parallelization Strategy: parallel sampling on a GPU or CPU cluster enables dramatically reduced wall clock time to reach the required target accuracy. 5) Numerical Integration: Higher-order integrators can improve accuracy at the cost of additional gradient evaluations per step.

This goal of this talk is to provide guidance to the optimal choice among these methods, which depends on specific application requirements including computational budget, accuracy demands, and problem dimensionality. Understanding the theoretical trade-offs enables practitioners to select and configure samplers that best match their particular constraints and objectives.

Thu, July 31 14:00–15:00

Saddlepoint Monte Carlo and its Application to Exact Ecological Inference

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In ecological inference, one wishes to model individual items, but perform inference based only on aggregate data. For instance, in two-round elections, we are interested the behaviour of individual voters, but only have access to aggregate vote numbers at each precinct. We develop an exact method for a large class of Ecological Inference Bayesian models, which scales to the large data setting. Our approach solves a more general problem: assuming X is a random vector and A a non-invertible matrix, one sometimes need to perform inference while only having access to samples of $Y = AX$. The corresponding likelihood is typically intractable. One may still be able to perform exact Bayesian inference using a pseudo-marginal sampler, but this requires an unbiased estimator of the intractable likelihood.

We propose saddlepoint Monte Carlo, a method for obtaining an unbiased estimate of the density of Y with very low variance, for any model belonging to an exponential family. Our method relies on importance sampling and characteristic functions, with insights brought by the standard saddlepoint approximation scheme with exponential tilting. We show that saddlepoint Monte Carlo makes it possible to perform exact inference on particularly challenging problems and datasets. We present a study of the carryover of votes between the two rounds of various French elections, using the finest available data (number of votes for each candidate in about 60,000 polling stations over most of the French territory).

We show that existing, popular approximate methods for ecological inference can lead to substantial bias; saddlepoint Monte Carlo is immune from this bias, and can handle ecological inference in the large data framework. We also present original results for the 2024 legislative elections on political centre-to-left and left-to-centre conversion rates when the far-right is present in the second round. Finally, we discuss other exciting applications for saddlepoint Monte Carlo in privacy and inverse problems, such as dealing with inference with empirical quantiles for continuous data.

[1] Voldoire T., Chopin N., Rateau G. and Ryder R.J. (2024). Monte Carlo and its Application to Exact Ecological Inference, *arxiv 2410.18243*, https://arxiv.org/abs/2410.18243,

Contributed Talks

Mon, July 28 10:30-12:30 Track E

Stereographic Multi-Try Metropolis Algorithms for Heavy-tailed Sampling

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We introduce a novel family of gradient-free Markov chain Monte Carlo (MCMC) algorithms that integrate the principles of multi-try Metropolis (MTM) and stereographic MCMC, designed specifically for efficient sampling of heavy-tailed distributions. Through scaling analysis and extensive simulations, we demonstrate that the proposed stereographic multi-try Metropolis (SMTM) algorithm outperforms both traditional Euclidean MTM and existing stereographic random-walk Metropolis. Furthermore, the SMTM algorithm has the potential to benefit from modern hardware, such as GPUs, allowing for improved performance through parallel implementation.

Mon, July 28 10:30-12:30 Track E

Creating rejection-free samplers by rebalancing skew-balanced jump processes

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Markov chain sampling methods form the backbone of modern computational statistics. However, many popular methods are prone to random walk behaviour, i.e. diffusion-like exploration of the sample space, leading to slow mixing that requires intricate tuning to alleviate. Non-reversible samplers can resolve some of these issues. We introduce a device that turns jump processes that satisfy a skew-detailed balance condition for a reference measure into a process that samples a target measure that is absolutely continuous with respect to the reference measure. This sampler is rejection-free, non-reversible and time-continuous. As an example, we apply the device to Hamiltonian dynamics discretized by the leapfrog integrator, resulting in a rejection-free non-reversible time-continuous version of Hamiltonian Monte Carlo (HMC). We prove the geometric ergodicity of the resulting sampler, and demonstrate its increased robustness to hyperparameter tuning compared to HMC through numerical examples. This comes at a computational cost at worst double that of HMC, in practice lower than other popular non-reversible samplers such as the Bouncy Particle Sampler.

Mon, July 28 10:30-12:30 Track E

Theoretical guarantees for lifted samplers

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The work I would like to present is about a particular class of Markov chain Monte Carlo (MCMC) methods which use non-reversible Markov chains commonly referred to as *lifted Markov chains*; the methods are commonly referred to as *lifted samplers*. The methods are not particularly new (they date back at least to Horowitz [1]), but they have recently been the subject of significant research work motivated by a general belief that, in statistical applications, they lead to more efficient estimators than their reversible counterparts which correspond to Metropolis–Hastings (MH) algorithms (see, e.g., Andrieu and Livingstone [2]). It was thus somewhat surprising to observe that it is not always the case in some recent work (see, e.g., Gagnon and Maire [3]). One can thus wonder what degree of inefficiency these chains may exhibit in worst-case scenarios. This is an important question given that lifted samplers are popular in practice, a consequence of the fact that they are often as easy to implement on a computer as their MH counterparts and often have the same computational complexity.

The main contribution of our work is to provide an answer to this question under arguably the most general framework. We proceed by leveraging the seminal work of Tierney [4] to define a lifted version of a generalized MH algorithm. Virtually any (reversible) MCMC method can be seen as a special case of this generalized MH algorithm, ranging from the traditional MH algorithm of Hastings [5] to the reversible jump algorithm of Green [6]. Our main theoretical result allows for a comparison between the generalized MH algorithm and its lifted version in terms of the variance of produced estimators. It essentially guarantees that the variance of estimators produced by the lifted version cannot be more than twice that of estimators produced by the generalized MH algorithm. This result indicates that, while there is potentially a lot to gain from lifting a Markov chain, there is not much to lose. We also show that our result is optimal, in the sense that it is not possible to improve on the factor 2 without additional assumptions. The definition of the lifted version of the generalized MH algorithm allows to understand how a lifted sampler can be constructed under such a general framework, which adds a methodological contribution to our theoretical contribution.

The efficiency of Markov chains is traditionally assessed by studying the characteristics of their Markov transition operators. To establish our theoretical result, we needed to connect the efficiency of two significantly different operators (those of the MH and lifted algorithms): in addition to not be defined on the same domain, one is self-adjoint while the other is not, which further complicates the analysis. One of our main achievements was to identify a specific auxiliary operator which acts a bridge and allows to connect the efficiency of the two aforementioned operators. This auxiliary operator is compared to the MH one through a Peskun ordering [7] established via a careful analysis of the Markov kernels, yielding sharp bounds. The connections between the MH and lifted algorithms is completed by comparing the auxiliary operator with the lifted one using a result in Andrieu and Livingstone [2].

[1] Horowitz, A. M. (1991) A generalized guided Monte Carlo algorithm. Phys. Lett. B, **268**, 247–252.

[2] Andrieu, C. and Livingstone, S. (2021) Peskun–Tierney ordering for Markovian Monte Carlo: Beyond the reversible scenario. Ann. Statist., **49**, 1958–1981.

[3] Gagnon, P. and Maire, F. (2024) An asymptotic Peskun ordering and its application to lifted samplers. Bernoulli, **30**, 2301–2325.

[4] Tierney, L. (1998) A note on Metropolis–Hastings kernels for general state spaces. Ann. Appl. Probab., **8**, 1–9.

[5] Hastings, W. K. (1970) Monte Carlo sampling methods using Markov chains and their applications. Biometrika, **57**, 97–109.

[6] Green, P. J. (1995) Reversible jump Markov chain Monte Carlo computation and Bayesian model determination. Biometrika, **82**, 711–732.

[7] Peskun, P. (1973) Optimum Monte-Carlo sampling using Markov chains. Biometrika, **60**, 607–612

Tue, July 29 10:30-12:30 Track E

Optimizing Generalized Hamiltonian Monte Carlo for Bayesian Inference applications

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In constrast to the widely adopted Hamiltonian/Hybrid Monte Carlo (HMC) [1], the Generalized Hamiltonian Monte Carlo (GHMC) algorithm [2, 3] leverages the irreversibility of its generated Markov chains, resulting in faster convergence to equilibrium and reduced asymptotic variance [4, 5].

Despite its theoretically predicted advantages, GHMC can be highly sensitive to the choice of a numerical integrator for the Hamiltonian equations and requires careful tuning of simulation parameters, such as the integration step size, the trajectory length, and the amount of random noise in momentum refreshment.

In this talk, we present a novel approach for finding optimal (in terms of sampling performance and accuracy) settings for a GHMC simulation. For an arbitrary simulated system, our methodology identifies a system-specific integration scheme that maximizes a conservation of energy for harmonic forces, along with appropriate randomization intervals for the simulation parameters, without incurring additional computational cost.

Numerical experiments on well-established statistical models exhibit, with the help of the state-of-the-art performance metrics, significant gains in GHMC sampling efficiency when

optimally tuned hyperparameters are chosen instead of heuristic or recommended ones. Comparative performance of GHMC and HMC with optimal settings is also discussed.

Additionally, we apply our methodology to three real-world case studies:

- Patient resistance to endocrine therapy in breast cancer;
- Influenza A (H1N1) epidemics outbreak;
- Modeling of cell-cell adhesion dynamics.

[1] Neal, Radford M. (2011). *MCMC Using Hamiltonian Dynamics*. Handbook of Markov Chain Monte Carlo (Eds: Brooks, S., Gelman, A., Jones, G., Meng, X.), Vol. 2 pp. 113–162. Chapman and Hall/CRC, New York.

[2] Horowitz, Alan M. (1991). *A generalized guided Monte Carlo algorithm*. Physics Letters B 268.2: 247–252.

[3] Kennedy, Anthony D. & Pendleton, Brian J. (2001). *Cost of the generalised hybrid Monte Carlo algorithm for free field theory*. Nuclear Physics B 607.3: 456–510.

[4] Ottobre, Michela (2016). *Markov Chain Monte Carlo and Irreversibility*. Reports on Mathematical Physics 77: 267–292.

[5] Duncan, Andrew B., Lelièvre, Tony & Pavliotis, Grigorios A. (2016). *Variance Reduction Using Nonreversible Langevin Samplers*. Journal of Statistical Physics 163: 457–491.

Tue, July 29 10:30-12:30 Track E

Bayesian Anomaly Detection in Variable-Order and Variable-Diffusivity Fractional Mediums

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Fractional diffusion equations (FDEs) are powerful tools for modeling anomalous diffusion in complex systems, such as fractured media and biological processes, where nonlocal dynamics and spatial heterogeneity are prominent. These equations provide a more accurate representation of such systems compared to classical models but pose significant computational challenges, particularly for spatially varying diffusivity and fractional orders. In this talk I will present a Bayesian inverse problem for FDEs in a 2-dimensional bounded domain with an anomaly of unknown geometric and physical properties, where the latter are the diffusivity and fractional order fields. To tackle the computational burden of solving dense and ill-conditioned systems, we employ an advanced finite-element scheme incorporating low-rank

matrix representations and hierarchical matrices. For parameter estimation, we implement two surrogate-based approaches using polynomial chaos expansions: one constructs a 7-dimensional surrogate for simultaneous inference of geometrical and physical parameters, while the other leverages solution singularities to separately infer geometric features, then constructing a 2-dimensional surrogate to learn the physical parameters and hence reducing the computational cost immensely. These surrogates are used inside a Markov chain Monte Carlo algorithm to infer the unknown parameters.

Tue, July 29 10:30-12:30 Track E

Theoretical Guarantees of Mean Field Variational Inference for Bayesian Principal Component Analysis

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In this talk, we will investigate mean field variational inference for Bayesian principal component analysis (BPCA). Despite the wide usage of mean field variational inference for the BPCA model, there exists remarkably little theoretical justification. I will talk about new results on the convergence guarantees of the iterative coordinate ascent variational inference (CAVI) algorithm for the BPCA model. In particular, we will show that under reasonable technical assumptions on the initialization, CAVI converges exponentially fast to a local optimum. An interesting connection between the CAVI algorithm for the BPCA model and power iteration, which is a popular iterative numerical algorithm for finding singular vectors of a given matrix, will also be discussed.

Tue, July 29 10:30-12:30 Track E

Bayesian Analysis of Latent Underdispersion Using Discrete Order Statistics

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Researchers routinely analyze count data using models based on a Poisson likelihood, for which there exist many analytically convenient and computationally efficient strategies for

posterior inference. A limitation of such models however is the equidsipersion constraint of the Poisson distribution. This restriction prevents the model's likelihood, and by extension its posterior predictive distribution, from concentrating around its mode. As a result, these models are parametrically bound to produce probabilistic predictions with high uncertainty, even in cases where low uncertainty is supported by the data. While count data often exhibits overdispersion *marginally*, such data may nevertheless be consistent with a likelihood that is underdispersed *conditionally*, given parameters and latent variables. Detecting conditional underdispersion, however, requires one to fit the "right" model and thus the ability to build, fit, and critique a variety of different models with underdispersed likelihoods. Towards this end, we introduce a novel family of models for conditionally underdispersed count data whose likelihoods are based on order statistics of Poisson random variables. More specifically, we assume that each observed count coincides with the j^{th} order-statistic of D latent i.i.d. Poisson random variables, where j and D are user-defined hyperparameters. To perform efficient MCMC-based posterior inference in this family of models, we derive a data-augmentation strategy which samples the other $D-1$ latent variables from their exact conditional, given the observed (j, D)-order statistic. By relying on the explicit construction of a Poisson order statistic, this data augmentation strategy can be modularly combined with the many existing inference strategies for Poisson-based models. We generalize this approach beyond the Poisson to any non-negative discrete parent distribution and, in particular, show that models based on negative binomial order statistics can flexibly capture both conditional under and overdispersion. To illustrate our approach empirically, we build and fit models to three real count data sets of flight times, COVID-19 cases counts, and RNA-sequence data, and we demonstrate how models with underdispersed likelihoods can leverage latent structure to make more precise probabilistic predictions. Although the possibility of conditional underdispersion is often overlooked in practice, we argue that this is at least in part due to the lack of tools for modeling underdispersion in settings where complex latent structure is present.

Fri, August 1 9:00–10:30 Track C

Monte Carlo simulation approach to solve distributed order fractional mathematical model

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This work presents a novel approach to solving time-distributed order fractional nonhomogeneous differential equations using the Monte Carlo simulation method. Fractional differential equations with distributed orders are critical for modeling complex systems with memory and hereditary effects, such as viscoelastic materials, anomalous diffusion, and biological processes. The inclusion of time-distributed orders introduces additional challenges in analytical and numerical solutions, especially in the presence of nonhomogeneous terms.

The proposed Monte Carlo method reformulates the distributed order fractional equation into an equivalent integral representation. By simulating random processes and utilizing probabilistic interpretations of fractional operators, the solution is computed as a average over numerous realizations. The flexibility of Monte Carlo simulations makes them particularly well-suited for addressing the inherent complexity of distributed order systems.

Numerical experiments validate the efficiency and effectiveness of the Monte Carlo approach, illustrating its capability to handle various distributed order kernels and nonhomogeneous terms. This method offers a robust, scalable, and versatile framework for solving fractional differential equations, paving the way for broader applications in science and engineering.

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[3] Kumar, Yashveer & Singh, Vineet Kumar (2021). *Compuational approach based on wavelets for financial mathematical model governed by distributed order time-fractional partial differential equation*. Mathematics and Computers in Simulation, 190, 531-569.

Fri, August 1 9:00–10:30 Track C

Benchmarking the Geant4-DNA 'UHDR' Example for Monte Carlo Simulation of pH Effects on Radiolytic Species Yields Using a Mesoscopic Approach

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Background and Aims
FLASH radiotherapy is an innovative cancer treatment technique that delivers high radiation doses in an extremely short time ($\geq$ 40 Gy/s), inducing the so-called FLASH effect—characterized by the sparing of healthy tissue while maintaining effective tumor control. However, the mechanisms underlying the FLASH effect remain unclear, and ongoing research aims to elucidate them. One approach to investigating this phenomenon is through Monte Carlo simulations of particle transport and the resulting radiolysis in aqueous media, enabling comparisons between FLASH and conventional irradiation.

Methods
To provide a useful tool for investigating the effects of FLASH irradiation, the Geant4-DNA example "UHDR" was introduced in the beta release 11.2.0 of Geant4 (June 2023). This example incorporates a newly developed radiolysis chemical stage based on the diffusion-reaction master equation (RDME), a mesoscopic method that bridges microscopic particle-level interactions and macroscopic chemical kinetics. This approach allows the extension of the simulation time to minutes post-irradiation, enabling the validation of equilibrium processes that may play a crucial role on long time scales. In this context, the impact of pH on radiolytic species yields towards equilibrium is particularly important. For the first time in Geant4-DNA, the UHDR example allows taking into account the effect of different pH values on water radiolysis.

Results
This study aims to benchmark the capability of the UHDR example to accurately reproduce the effect of pH on radiolytic species yields. Preliminary results are currently under analysis for 1 MeV electron and 300 MeV proton irradiation in the conventional modality, with comparisons against literature data.

Conclusions
The ability to simulate the impact of pH on water radiolysis represents a significant advancement in studying the evolution of radiolytic species toward equilibrium. This improvement could provide valuable insights into potential differences in chemical evolution under FLASH irradiation compared to conventional irradiation.

Fri, August 1 9:00–10:30 Track C

Multilevel simulation of ensemble Kalman methods: interactions across levels

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To solve problems in domains such as filtering, optimization, and posterior sampling, ensemble Kalman methods have recently received much attention. These parallelizable and often gradient-free algorithms use an ensemble of particles that evolve in time, based on a combination of well-chosen dynamics and interaction between the particles. For computationally expensive dynamics, the cost of attaining a high accuracy quickly becomes prohibitive. To improve the asymptotic cost-to-error relation, different multilevel Monte Caro techniques have been proposed. These methods simulate multiple differently sized ensembles at different resolutions, corresponding different accuracies and costs. While particles within one of these ensembles do interact with each other, a key question is whether and how particles should interact across ensembles and levels. In this talk, we will outline and compare the most common approaches to such multilevel ensemble interactions.

Fri, August 1 9:00–10:30 Track C

Adaptive Max-EWMA Control Chart with SVR: Monte Carlo Simulation for Run Length Analysis

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In industrial quality control, monitoring process variations is crucial for ensuring product reliability, particularly when dealing with non-normal data distributions. This study proposes an adaptive Max-EWMA control chart integrated with Support Vector Regression (SVR) for the simultaneous monitoring of process mean and variance. The approach utilizes a dynamic smoothing constant predicted by SVR to enhance sensitivity to real-time process shifts. To address non-normality, Weibull-distributed data is transformed into a standard normal form before analysis. The performance of the proposed method is extensively evaluated through Monte Carlo simulations to assess the run length profile under different process shift scenarios. Results demonstrate the effectiveness of the approach in detecting small to moderate shifts, with the linear kernel exhibiting superior balance between sensitivity and stability, making it an optimal choice for industrial applications. The findings highlight the robustness of the proposed control chart and its adaptability in real-time process monitoring.

Mon, July 28 15:30–17:30 Track I

Halton Sequences, Scrambling and the Inverse Star-Discrepancy

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Halton sequences are classical examples of multi-dimensional low-discrepancy sequences. Braaten and Weller discovered that scrambling strongly reduces their empirical star-discrepancy. A similar approach may be applied to certain multi-parameter subsequences of Halton sequences. Indeed, results from p-adic analysis guarantee that these subsequences still have the theoretical low-discrepancy property while scrambling has strong effects on the empirical star-discrepancy. By optimizing the parameters of these subsequences known empiric bounds for the inverse star-discrepancy can be improved.

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Mon, July 28 15:30–17:30 Track I

Star discrepancy and uniform approximation under weighted simple and stratified random sampling

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We mainly consider two problems in this talk. First, We consider random discrepancy under weighted importance sampling of a class of stratified input. We give the expected L_p-discrepancy$(2 \leq p < \infty)$ upper bound in weighted form under a class of stratified sampling. This result contributes to the error estimate of the upper bound of the integral approximation under weighted importance sampling, and and our sampling pattern is a stratified input. Second, we discuss the probabilistic star discrepancy for a random double infinite matrix and propose an improvement to the coefficient of an existing result, we mainly use the optimal refined $\delta-$bracketing number so far.

[1] J. Dick, D. Rudolf and H. Zhu. (2019). A weighted discrepancy bound of quasi-Monte

Carlo importance sampling. Statist. Probab. Lett., 100-106.

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Mon, July 28 15:30–17:30 Track I

Transport Quasi-Monte Carlo

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Quasi-Monte Carlo (QMC) is a powerful method for evaluating high-dimensional integrals. However, its use is typically limited to distributions where direct sampling is straightforward, such as the uniform distribution on the unit hypercube or the Gaussian distribution. For general target distributions with potentially unnormalized densities, leveraging the low-discrepancy property of QMC to improve accuracy remains challenging. We propose training a transport map to push forward the uniform distribution on the unit hypercube to approximate the target distribution. Inspired by normalizing flows, the transport map is constructed as a composition of simple, invertible transformations. To ensure that RQMC achieves its superior error rate, the transport map must satisfy specific regularity conditions. We introduce a flexible parametrization for the transport map that not only meets these conditions but is also expressive enough to model complex distributions. Our theoretical analysis establishes that the proposed transport QMC estimator achieves faster convergence rates than standard Monte Carlo, under mild and easily verifiable growth conditions on the integrand. Numerical experiments confirm the theoretical results, demonstrating the effectiveness of the proposed method in Bayesian inference tasks.

Mon, July 28 15:30–17:30 Track I

Using Normalizing Flows for Efficient Quasi-Random Sampling for Copulas

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In finance and risk management, copulas are used to model the dependence between stock

prices and insurance losses to compute expectations of interest. Generally, Monte Carlo (MC) sampling is used to generate copula samples to approximate expectations. To reduce the variance of the approximation, we can use quasi-Monte Carlo (QMC) sampling to generate copula samples. This paper examines a new method to generate quasi-random samples from copulas requiring fewer training resources than previous methods such as the generative moment matching networks (GMMN) model [1]. Traditional methods that do not use generative models often rely on conditional distribution methods (CDM) to generate quasi-random samples from specific copulas [2]. CDM is limited to only a few parametric copulas (Gumbel has no efficient CDM to sample quasi-random samples) in low dimensions [2]. Here, we propose using a powerful and simple generative model called Normalizing Flows (NFs) to generate quasi-random samples for any copula, including cases where we only have data available. NFs are a type of explicit generative model that relies on transforming a simple density, such as a normal density, through efficient invertible transformations that rely on the change of variables formula into a density that models complex data that facilitates easy sampling and efficient inverting of samples from complex data to normal data and vice versa. The benefit of these NFs for copula modelling is that their training is efficient in terms of runtime, allowing for larger batch sizes compared to the GMMN model [1]. Also, it is sample-efficient; it only needs samples from the copula and not samples from the normal as the GMMN model [1] required. Once the NF model is trained, we can efficiently invert the model to take as input quasi-random samples to generate quasi-random copula samples. Through many different simulations and applications, we show our approach allows us to leverage the benefit of QMC in a variety of real-world settings involving dependent data.

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Tue, July 29 15:30-17:30 Track J

Approximation using median lattice algorithms

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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.

Tue, July 29 15:30-17:30 Track J

Convergence Rates of Randomized Quasi-Monte Carlo Methods under Various Regularity Conditions

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In this work, we analyze the convergence rate of randomized quasi-Monte Carlo (RQMC) methods under Owen's boundary growth condition (Owen, 2006) via spectral analysis. We examine the RQMC estimator variance for two commonly studied sequences—the lattice rule and the Sobol' sequence—using the Fourier transform and Walsh–Fourier transform, respectively. Under certain regularity conditions, our results reveal that the asymptotic convergence rate of the RQMC estimator's variance closely aligns with the exponent specified in Owen's boundary growth condition for both sequence types. We also provide an analysis for certain discontinuous integrands.

In addition, we investigate the L^p integrability of weak mixed first-order derivatives of the integrand and study the convergence rates of scrambled digital nets. We demonstrate that the generalized Vitali variation with parameter $\alpha \in \left[\frac{1}{2}, 1\right]$ from Dick and Pillichshammer (2010) is bounded above by the L^p norm of the weak mixed first-order derivative, where $p = \frac{2}{3-2\alpha}$. Consequently, when the weak mixed first-order derivative belongs to L^p for $1 \leq p \leq 2$, the variance of the scrambled digital nets estimator converges at a rate of $\mathcal{O}\left(N^{-4+\frac{2}{p}} \log^{s-1} N\right)$. Together, these results provide a comprehensive theoretical framework for understanding the convergence behavior of RQMC methods and scrambled digital nets under various regularity assumptions.

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Tue, July 29 15:30-17:30 Track J

Use of rank-1 lattices in the Fourier neural operator

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The "Fourier neural operator" [2] is a variant of the "neural operator". Its defining characteristic, compared to the regular neural operator, is that it transforms the input to the Fourier domain at the start of each layer. This transformation uses the d-dimensional FFT on a regular grid in d dimensions. We describe how to do this more efficiently using rank-1 lattice points, which allow for a one-dimensional FFT algorithm, see, e.g., [1].

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Tue, July 29 15:30-17:30 Track J

Investigating the Optimum RQMC Batch Size for Betting and Empirical Bernstein Confidence Intervals

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The Betting [1] and Empirical Bernstein (EB) [1,2] confidence intervals (CIs) are finite sample (non-asymptotic) and require IID samples. Since both are non-asymptotic, they are much wider than confidence intervals based on the Central Limit Theorem (CLT) due to the stronger coverage property they provide. To apply these finite sample CIs to randomized quasi-Monte Carlo (RQMC), we take R independent replications of n RQMC points, averaging the n function evaluations within each replication. Given a fixed budget $N = nR$, we investigate the optimal n that minimizes the CI widths for both methods.

Using the code from [1], we ran simulations on various integrands (smooth, rough, one-dimensional, multi-dimensional) and ridge functions. Interestingly, the optimal n was quite small compared to N, often just 1 (plain IID), 2, or 4 when $N = 2^{10}$. Moreover, the optimal n appeared to grow quite slowly as N increased. Notably, both CI methods applied to RQMC

outperformed plain IID when the optimal n is greater than 1.

This experimental trend aligns with our analysis of Bennett's inequality for EB [2], which suggests that the optimum n is $O(N^{1/(2\theta+1)})$ for $\theta > 1/2$. Specifically, for $\theta = 3/2$, which occurs for smoother integrands, we obtain $n = O(N^{1/4})$. For $\theta = 1$, which corresponds to a typical Koksma-Hlawka rate, we get $n = O(N^{1/3})$. The ratio of RQMC EB CI widths to plain IID EB CI widths is $\Theta(N^{(1-2\theta)/(4\theta+2)})$. For $\theta = 1$, we get a ratio of $\Theta(N^{-1/6})$, while for $\theta = 3/2$, we get a more favorable width ratio of $\Theta(N^{-1/4})$.

On the other hand, CLT based CIs using RQMC are only asymptotically valid. The value of R could be any reasonable number that isn't too small, and remains constant as the total sample size, N, increases. This means that $n = \Theta(N)$, which takes full advantage of the power of QMC. It is also important to note that both Betting and EB require the random variables to be bounded between 0 and 1, unlike CLT based CIs.

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Wed, July 30 10:30-12:30 Track E

Sampling with constraints

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We will present first order and second order numerical integrators for reflected (overdamped) Langevin dynamics [1] and confined (underdamped) Langevin dynamics [2], respectively. We show how these SDEs can be used for sampling from a desired measure with compact support. We will also discuss sampling on hyper-surfaces. We will showcase numerical examples to verify the presented results.

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Wed, July 30 10:30-12:30 Track E

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Hamiltonian Monte Carlo (HMC) is widely used for sampling from high-dimensional target distributions with probability density known up to proportionality. While HMC possesses favorable dimension scaling properties, it encounters challenges when applied to strongly multimodal distributions. Traditional tempering methods, commonly used to address multimodality, can be difficult to tune, particularly in high dimensions. In this study, we propose a method that combines a tempering strategy with Hamiltonian Monte Carlo, enabling efficient sampling from high-dimensional, strongly multimodal distributions. Our approach involves proposing candidate states for the constructed Markov chain by simulating Hamiltonian dynamics with time-varying mass, thereby searching for isolated modes at unknown locations. Moreover, we develop an automatic tuning strategy for our method, resulting in an automatically-tuned, tempered Hamiltonian Monte Carlo (ATHMC). Unlike simulated tempering or parallel tempering methods, ATHMC provides a distinctive advantage in scenarios where the target distribution changes at each iteration, such as in the Gibbs sampler. We numerically show that our method scales better with increasing dimensions than an adaptive parallel tempering method and demonstrate its efficacy for a variety of target distributions, including mixtures of log-polynomial densities and Bayesian posterior distributions for a sensor network self-localization problem.

Wed, July 30 10:30-12:30 Track E

Localized consensus-based sampling for non-Gaussian distributions

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Drawing samples distributed according to a given unnormalized probability density function is a common task in Bayesian inverse problems. Algorithms based on an ensemble of interacting *particles*, moving in parameter space, are gaining in popularity for these problems since they are often parallelizable, derivative-free, and affine-invariant. However, most are only accurate for near-Gaussian target distributions; an example is the consensus-based sampling (CBS) method [1]. We propose a novel way to derive CBS from ensemble-preconditioned Langevin diffusions by first approximating the target potential by its anisotropic Moreau envelope, then approximating the proximal operator by a weighted mean, and finally assuming that the initial and target distributions are Gaussian. We adapt these approximations with non-Gaussian distributions in mind and arrive at a new interacting-particle method for sampling, which we call *localized consensus-based sampling*. Numerical tests illustrate that localized CBS compares favorably to alternative methods in terms of affine-invariance and performance on non-Gaussian distributions.

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Wed, July 30 10:30-12:30 Track E

Importance Sampling for Hawkes Processes

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In 1971, Alan Hawkes [1] introduced a highly influential point process N for which, given a constant $\mu > 0$ and a $[0, \infty)$-valued function g, the intensity process X takes the form,

$$X_t = \mu + \int_0^t g(t-s)\,\mathrm{d}N_s\,, \quad (t \geq 0)\,. \tag{2.1}$$

By now, Hawkes processes have found a wide array of application in the sciences, engineering, statistics, operations research, mathematical finance and machine learning. We develop importance sampling estimators for rare-event probabilities of the form $\mathbb{P}(N_t \geq c\,t)$ and

general functions g in (2.1). This problem has received little attention to date, as for most g, the process (N, X) is non-Markovian and lends to little mathematical tractability. Our approach is based on a Girsanov change of intensity coupled with a conditioning on the rare-event. We prove asymptotic optimality of the resulting importance sampling estimators in the limit $t \to \infty$. Related large deviations results and an extension to fully nonlinear models of N with intensity $\phi(X)$ are presented. Numerical simulations illustrate the performance of our importance sampling estimators relative to Monte Carlo for various functions g as well as to exponential tilting in the case of an exponential g (the sole tractable model).

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Thu, July 31 15:30–17:30 Track I

Revisiting the Gibbs Sampler: A Conditional Modeling Perspective

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The Gibbs sampler (GS) is a fundamental algorithm for approximating analytically intractable distributions. Two major generalizations of GS are the partially collapsed Gibbs sampler (PCGS) and the pseudo-Gibbs sampler (PGS). For PCGS, the associated Markov chain is heterogeneous with varying state spaces, making traditional convergence analysis challenging. To address this, we introduce the iterative conditional replacement (ICR) algorithm and prove its convergence. Furthermore, ICR provides a systematic approach for approximating multiple stationary distributions arising in PGS. Our approach emphasizes the advantage of treating each conditional density with its own operator, rather than aggregating all conditionals into a single operator.

Thu, July 31 15:30–17:30 Track I

Concatenation of Markov processes for Monte Carlo Integration

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Markov Chain Monte Carlo (MCMC) is a sophisticated sampling technique used to sample from a probability distribution when conventional methods are impractical. Widely applied in statistics, machine learning, physics, and finance, MCMC generates samples from a probability distribution through an invariant Markov process. However, controlling and fine-tuning the process pose challenges, particularly in achieving both rapid local exploration and global distribution discovery. The Metropolis-Hastings algorithm, the most popular MCMC technique, while practical, struggles to excel in these objectives due to its inherent reversibility, leading to diffusive exploration and the need for large-scale perturbations for global discovery.

Wang et al. [2] introduced a novel MCMC approach, which is based on the concatenation of Markov processes [1]. It allows the usage of an essentially arbitrary Markov process for local exploration. That way, the process can be chosen to satisfy a desired exploration behavior suitable for the state space at hand without worrying about invariance at this point. The process is executed up to a certain finite lifetime. After this time has elapsed, the process is *killed* and started afresh at a spawn location drawn from a *regeneration* distribution. The lifetime is chosen in a way ensuring that the overall process is invariant with respect to a given target distribution.

We generalize this idea and introduce it with appropriate rigor. We show how the validity of the method can be established for a more general class of Markov processes. We also allow the usage of a whole family of Markov processes for local exploration with possibly varying exploration characteristic. We establish a transfer mechanism between consecutive processes, which allows the user to specify the initial state of the newly spawned process to depend on the exit point of the previous one. Not least, we derive a Rao-Blackwellization technique which guarantees variance reduction in practice. We showcase the potential of the framework in a practical rendering experiment. We compare the method proposed in [2] with existing methods based on Metropolis-Hastings algorithms with Random-Walk, Langevin and Hamiltonian proposals, respectively.

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Thu, July 31 15:30–17:30 Track I

Polynomial approximation for efficient transport-based sampling

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Sampling from non-trivial probability distributions is a fundamental challenge in uncertainty quantification and inverse problems, particularly when dealing with high-dimensional domains, costly-to-evaluate or unnormalized density functions, and non-trivial support structures. Measure transport via polynomial density surrogates [1] provides a systematic and constructive solution to this problem by reformulating it as a convex optimization task with deterministic error bounds. This approach is particularly efficient for smooth problems but can become computationally demanding when dealing with highly concentrated posterior distributions, as constructing the density surrogate requires many evaluations in regions where the density is nearly zero—leading to an inefficient allocation of computational resources. In this talk, we explore how the computational cost in such cases can be further reduced by first approximating the potential function with a polynomial. This additional approximation step shifts the focus of expensive evaluations toward capturing the underlying system more effectively. The surrogate-based posterior can then be evaluated cheaply and approximated with high accuracy, enabling efficient transport-based sampling. We discuss the implications of this strategy and examine its potential to enhance performance in demanding inference problems.

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Thu, July 31 15:30–17:30 Track I

Fast Approximate Matrix Inversion via MCMC for Linear System Solvers

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A key prerequisite of modern iterative solvers of linear algebraic equations $Ax = b$ is the fast computation of a pre-conditioner matrix P that gives a good approximation to the (generalized) inverse of A such that the set of equations obtained by pre-multiplying with P, $PAx = Pb$, is solved quickly. We study the classical Ulan-von Neumann MCMC algorithm that was designed based on the Neumann infinite series representation of the inverse of a non-singular matrix. The parameters of the MCMC algorithm determine the overall time to solve

$Ax = b$, which is a metric that reflects both the time to compute the MCMC preconditioner P and its quality as a preconditioner to solve the linear equations. Our main focus is on how the MCMC parameters should be tuned to speed up computations in applications that require repeated calls to the solver with varying matrices A, a common scenario for instance in numerical approximations of physical phenomena. We present a model that relates key features of matrices A with good choices of MCMC algorithm parameters that lead to a fast overall time to find a solution to $Ax = b$. A computationally efficient approach based on Bayesian experimental design is described to learn and update this model while minimizing the number of runs of the expensive solver in application settings that solve of linear system over well defined sets of A matrices. We present numerical experiments to illustrate the efficacy of this approach. In another contribution, we present a new MCMC algorithm which we term as *regenerative Ulam-von Neumann* algorithm. It exploits a regenerative structure present in the Neumann series that underlies the original algorithm and improves on it by producing an unbiased estimator of the matrix inverse. A rigorous analysis of performance of the algorithm is provided. This includes the variance of the estimator, which allows one to estimate the time taken to obtain solutions of a desired quality. Finally, numerical experiments verify the qualitative effectiveness of the proposed scheme.

Thu, July 31 10:30–12:30 Track D

The Stochastic Differential Equations of the Heston Model for Option Pricing

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The Heston model is a widely used stochastic volatility model for option pricing, addressing the limitations of the Black-Scholes model by incorporating a stochastic variance process. This talk will cover the stochastic differential equations (SDEs) governing the Heston model, demonstrating their application in option pricing.

The Heston model introduces a stochastic process for volatility, improving the accuracy of derivative pricing. The dynamics of the asset price S_t and its variance v_t under the Heston model are given by[1]:

$$dS_t\& = \mu S_t dt + \sqrt{v_t} S_t dW_t^S, \tag{2.2}$$
$$dv_t\& = \kappa(\theta - v_t)dt + \sigma\sqrt{v_t} dW_t^v, \tag{2.3}$$

where:

- μ is the drift of the asset price.
- κ is the rate of mean reversion of variance v_t towards long-term mean θ.
- σ represents the volatility of volatility.

- dW_t^S and dW_t^v are Wiener processes with correlation ρ.

We will explore Monte Carlo methods as a numerical approach to simulate price paths and compute option prices for European and American derivatives [2],[3]. Furthermore, an interactive Shiny web application will be presented, showcasing real-time simulations and visualizations of option pricing under the Heston framework.

An interactive web-based application is implemented using Shiny in R, enabling users to:

- Adjust input parameters $(S_0, K, r, T, \mu, \theta, \kappa, \sigma, \rho)$.
- Perform Monte Carlo simulations to compute option prices.
- Visualize option price distributions and convergence results.

The Shiny application offers an interactive tool for financial analysis. Future work may explore enhancements such as incorporating jump-diffusion models and GPU-accelerated simulations.

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Thu, July 31 10:30–12:30 Track D

Characterizing Efficacy of Geometric Brownian Motion Expectation-based Simulations on Low-Volatility American Common Stocks

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In this manuscript, daily, monthly, and annual geometric Brownian motion forecasts are obtained and tested for reliability upon 21 stock symbols within NASDAQ of varying volatilities and drifts. Biweekly, monthly, biannual, and annual rolling windows were used as a preliminary filtering scheme to remove unreliable stock symbols, and then accuracy was further evaluated on stocks with higher accuracies in the first screening. Annual and 10-year windows were used to estimate the drift and diffusion component and then applied to obtain one-period-ahead geometric Brownian motion stock values and associated probabilities. Further building off of these one-period-ahead values, expected values for 1-252 periods were estimated. Expected values of each stock were estimated by totaling up the product of the stock value and its associated probabilities, and tested over multiple rolling-windows for

reliability. The results indicate that geometric Brownian-simulated expected index values estimated using one thousand simulations can be slightly reliable if catered and re-optimized to specific stock characterizations, but only for a daily window, and even then only slightly preferable to flipping a coin. Expected values estimated with less than 100 simulations were thrown out, seen as unreliable.

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Thu, July 31 10:30–12:30 Track D

Efficient Pricing for Variable Annuity via Simulation

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Variable Annuities (VAs) are insurance products that offer policyholders exposure to financial market upside potential while safeguarding against downside risk through optional riders, such as Guaranteed Minimum Death Benefits (GMDBs), Guaranteed Minimum Accumulation Benefits (GMABs), and Guaranteed Minimum Withdrawal Benefits (GMWBs). These riders, tailored to policyholders' needs, introduce a complex risk profile combining mortality and financial uncertainties, rendering VA pricing and fee determination computationally challenging. Due to this complexity, Monte Carlo simulation is often the only practical approach for valuing these contracts.

In this study, we address the problem of setting fair management fees for VA rider combinations using the equivalence principle, which balances the expected present value of premiums and benefits. We formulate fee determination as a stochastic root-finding problem, expressed as

$$E[V(\varphi)] - P = 0,$$

where $E[V(\varphi)]$ denotes the expected present value of VA benefits under fee structure φ, and P represents the premium. The VA benefit $V(\varphi)$ reflects the evolution of the contract's shadow account value and various benefit guarantees over the contract's lifetime. As a result, estimating its expected value is computationally challenging. Moreover, solving the root-finding problem requires estimating the gradient of this expectation. To solve this, we employ stochastic gradient estimation techniques, such as finite differences and infinitesimal perturbation analysis (IPA). We analyze the theoretical properties and computational performance of the proposed root-finding algorithms, offering insights into their efficacy for VA pricing. Our results show that gradient estimation techniques have a significant impact on the efficiency and accuracy of estimating fair fees for various rider combinations.

Fri, August 1 9:00–10:30 Track D

Revisiting self-normalized importance sampling: new methods and diagnostics

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Importance sampling (IS) can often be implemented only with normalized weights, yielding the popular self-normalized IS (SNIS) estimator. However, proposal distributions are often

learned and evaluated using criteria designed for the unnormalized IS (UIS) estimator.

In this talk, we aim to present a unified perspective on recent methodological advances in understanding and improving SNIS. We propose and compare two new frameworks for adaptive importance sampling (AIS) methods tailored to SNIS. Our first framework exploits the view of SNIS as a ratio of two UIS estimators, coupling two separate AIS samplers in a joint distribution selected to minimize asymptotic variance. Our second framework instead proposes the first MCMC-driven AIS sampler directly targeting the (often overlooked) optimal SNIS proposal.

We also establish a close connection between the optimal SNIS proposal and so-called subtractive mixture models (SMMs), where negative coefficients are possible - motivating the study of the properties of the first IS estimators using SMMs.

Finally, we propose new Monte Carlo diagnostics specifically for SNIS. They extend existing diagnostics for numerator and denominator by incorporating their statistical dependence, drawing on different notions of tail dependence from multivariate extreme value theory.

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Fri, August 1 9:00–10:30 Track D

Quantitative results on sampling from quasi-stationary distributions

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We study the rate of convergence of Sequential Monte Carlo (SMC) methods for approximating the quasi-stationary ditribution (QSD) of Markov processes. For processes with killing or absorption, the QSD appears as a stable behavior observed before extinction, or as the limiting distribution of the process conditioned on not being absorbed. We give quantitative lower and upper bounds for the particle filter approximation of these distributions. For the lower bound, we show that fast mixing is not enough to guarantee that simulation methods

can converge in few steps. In the upper bound, we show that SMC with adaptive resampling has a rate depending on the number of steps, the mixing time, and in how fast the processed gets killed. Our seems to be the first result to have a quantitative dependency of this form that is valid for discrete time Markov chains in general state spaces. Our techniques and concentration results for bounding the approximations of SMC with adaptive resampling are also novel, and we believe might be applicable in other scenarios that can benefit from the lower variance obtained due to an adaptive approach.

Fri, August 1 9:00–10:30 Track D

Serial ensemble filtering with marginal coupling

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Serial filtering refers to a univariate, state by state Bayesian inference problem. Extant methods for serial filtering result in suboptimal posterior samples for severely non-Gaussian, multimodal inference settings. We fix this problem by rigorously coupling the state marginal densities with information about their joint density. This formulation allows for accurately sampling the Bayesian posterior across a variety of challenging text problems.

Wed, July 30 14:00–16:00 Track J

Stochastic gradient Langevin dynamics with non-stationary data

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We investigate the mixing properties of the stochastic gradient Langevin dynamics (SGLD) algorithm with a fixed step size. While most existing studies on SGLD assume an i.i.d. data stream, this assumption is often unrealistic in practical applications, such as financial time series analysis, natural language processing, and sensor data processing. In such settings, the sequence of iterates no longer forms a Markov chain, significantly complicating the

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mathematical analysis [1, 2].

To address this challenge, we model the iterates as a Markov chain in a random environment (see [4, 5], and [6]). Under standard dissipativity and Lipschitz conditions, we establish the transfer of α-mixing properties from the data stream to the sequence of iterates [3]. This enables us to derive key theoretical results, including the law of large numbers, the central limit theorem, and concentration inequalities for SGLD in the non-convex setting. Our findings provide theoretical guarantees for SGLD in a more realistic scenario where the data merely weakly dependent.

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Wed, July 30 14:00–16:00 Track J

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In this article, we study the problem of sampling from distributions whose densities are not necessarily smooth nor log-concave. We propose a simple Langevin-based algorithm that does not rely on popular but computationally challenging techniques, such as the Moreau Yosida envelope or Gaussian smoothing. We derive non-asymptotic guarantees for the convergence of the algorithm to the target distribution in Wasserstein distances. Non asymptotic bounds are also provided for the performance of the algorithm as an optimizer, specifically for the solution of associated excess risk optimization problems.
Possible extensions to potentials with log-gradients that grow super-linearly may also be discussed.

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

[1] Johnston, T., Lytras, I., Makras, N., Sabanis, S. (2025). The Performance Of The Unadjusted Langevin Algorithm Without Smoothness Assumptions. arXiv preprint arXiv:2502.03458.

Wed, July 30 14:00–16:00 Track J

Langevin-based strategies for nested particle filters

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Many problems in some of the most active fields of science require to estimate parameters and predict the evolution of complex dynamical systems using sequentially collected data. The nested particle filter (NPF) framework stands out since it is the only fully recursive probabilistic method for Bayesian inference. That is, it computes the joint posterior distribution of the parameters and states while maintaining a computational complexity of $\mathcal{O}(T)$, which makes it particularly suitable for long observation sequences.

A key strategy to keep particle diversity in the parameter space, given the static nature of the parameters, is jittering. The parameter space is explored by perturbing a subset of particles with arbitrary variance or applying a controlled variance to all particles. As the perturbations are controlled, it ensures convergence to the true posterior distribution while keeping the full framework recursive. However, this is not an efficient exploration strategy, particularly for problems with a higher dimension in the parameter space.

To address this limitation, we propose a Langevin-based methodology within the NPF framework. A challenge is that the required score function is intractable. We propose to approximate the score with an accurate method that is provably stable over time, and to explore strategies to reduce its computational cost while retaining accuracy. This approach significantly improves the scalability of NPF in the parameter dimension, while still ensuring asymptotic convergence to the true posterior, as well as maintaining computational feasibility.

Wed, July 30 14:00–16:00 Track J

Taming the Interacting Particle Langevin Algorithm – The Superlinear Case

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Recent advances in stochastic optimization have yielded the interacting particle Langevin algorithm (IPLA), which leverages the notion of interacting particle systems (IPS) to efficiently sample from approximate posterior densities. This becomes particularly crucial in relation to the framework of Expectation-Maximization (EM), where the E-step is computationally challenging or even intractable. Although prior research has focused on scenarios involving convex cases with gradients of log densities that grow at most linearly, our work extends this framework to include polynomial growth. Taming techniques are employed to produce an explicit discretization scheme that yields a new class of stable, under such non-linearities, algorithms which are called tamed interacting particle Langevin algorithms (tIPLA). We obtain non-asymptotic convergence error estimates in Wasserstein-2 distance for the new class under the best known rate.

[1] Tim Johnston, Nikolaos Makras and Sotirios Sabanis, *Taming the Interacting Particle Langevin Algorithm – The Superlinear Case* (2024). Preprint: arxiv:2403.19587

Thu, July 31 15:30-17:30 Track J

Dynamical Low-Rank Approximation for SDEs: an interacting particle-system ROM

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Coauthor(s): Dr. Yoshihito Kazashi, Prof. Fabio Nobile

The Dynamical Low-Rank Approximation (DLRA) technique is a time-dependent reduced-order model (ROM) known for its significant advantages in terms of computational time and accuracy. Its appeal in uncertainty quantification is due to the fact that its solution is composed of time-dependent deterministic and stochastic bases, allowing the approximation to better track the dynamics of the studied system. In the context of stochastic differential equations (SDEs) a rigorous mathematical setting was presented in [1], using the so-called Dynamically Orthogonal (DO) framework. The well-posedness of this setting is nontrivial due to the coupled nature of the DO system: for instance, the deterministic basis depends on all stochastic basis paths, and the equations involve the inversion of a Gramian matrix.

When coming to stochastic discretization through a Monte-Carlo procedure, these features imply to deal with a interacting noisy particle dynamics. We proposed two fully discretized schemes based on the Monte-Carlo method, investigating their errors and analyzing possible issues arisen by the discretization of the Gramian inverse [2]. Theoretical results will be supported by numerical simulations.

[1] Yoshihito Kazashi, Fabio Nobile, and Fabio Zoccolan. *Dynamical low-rank approximation for stochastic differential equations*. Mathematics of Computation (2024).

[2] Yoshihito Kazashi, Fabio Nobile, and Fabio Zoccolan. *Numerical Methods for Dynamical low-rank approximation of stochastic differential equations, Part I & II*, in preparation (2025).

Thu, July 31 15:30-17:30 Track J

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Stochastic differential equations driven by Lévy processes have become established as models to describe the evolution of random variables such as financial and economic variables and more recently of climate variables, when the stochastic system shows jump discontinuities. In this talk, we derive a novel series representation of the flowmap of such stochastic differential equations in terms of commutators of vector fields with stochastic coefficients, in other words a Chen–Strichartz formula. We provide an explicit expression for the components in this series. Our results extend previous results for deterministic and continuous stochastic differential equations.

Thu, July 31 15:30-17:30 Track J

Comparing Probabilistic Load Forecasters: Stochastic Differential Equations and Deep Learning

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Generating probabilistic predictions for the electricity-load profile is the foundation of efficient use of renewable energy and diminishing carbon footprint.

In this talk, we consider the problem of creating probabilistic forecasts of the day-ahead electricity consumption profile of an agglomerate of buildings in the city of Lausanne (Switzerland) in the absence of an externally provided prediction function.

We propose a nonparametric, data-driven, approach based on Itô' Stochastic Differential Equations (SDEs) [1]. Our work is novel in that the mean function of the SDE is expanded on a Fourier periodic basis, capturing intra-day and intra-week periodic features. Using a derivative tracking term, we impose the trajectories of the process to revert toward the mean. To model high-volatility levels associated with more uncertain electricity consumption regimes, we employ a square-root type diffusion coefficients.

Maximum-Likelihood estimation is used to infer the parameters of the model coherently with the available observations of the time history. We show that the maximization problem is well posed and that it admits at least one solution over the feasible domain.

We compare the probabilistic predictions generated by the SDE with Deep Learning based probabilistic forecaster. On the one hand, we introduce a Deep Learning forecaster based on Long short-term memory (LSTM) recurrent neural networks trained by minimizing the quantile loss function. This approach allows the generation of confidence intervals by sampling from the one-step-ahead univariate cumulative density function (CDF) associated with the electricity consumption of the future time instant. On the other hand, inspired by [2], we consider Multivariate Quantile Function Forecasters that, based on Normalizing Flows, learn the multivariate cumulative density function of the day-ahead electricity consumption.

Metrics such as Continuous ranked probability score and Prediction interval coverage percentage are used to assess the quality of the forecasts.

We show that SDEs generate reliable and interpretable predictions while presenting the most parsimonious and computationally efficient structure among the three models.

[1] Riccardo Saporiti, Fabio Nobile, Celia García-Pareja. *Probabilistic Forecast of the Day-Ahead electricity consumption profile with Stochastic Differential Equations: a comparison with Deep Learning models*. In preparation.

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Thu, July 31 15:30-17:30 Track J

Forward Propagation of Low Discrepancy Through McKean–Vlasov Dynamics: From QMC to MLQMC

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This work develops a particle system addressing the approximation of McKean–Vlasov stochastic differential equations (SDEs). The novelty of the approach lies in involving low discrepancy sequences nontrivially in the construction of a particle system with coupled noise and initial conditions. Weak convergence for SDEs with additive noise is proven. A numerical study demonstrates that the novel approach presented here doubles the respective convergence rates for weak and strong approximation of the mean-field limit, compared with the standard particle system. These rates are proven in the simplified setting of a mean-field ordinary differential equation in terms of appropriate bounds involving the star discrepancy for low discrepancy sequences with a group structure, such as Rank-1 lattice points. This construction nontrivially provides an antithetic multilevel quasi-Monte Carlo estimator. An asymptotic error analysis reveals that the proposed approach outperforms methods based on the classic particle system with independent initial conditions and noise.

Mon, July 28 15:30-17:30 Track J

A probabilistic Numerical method for semi-linear elliptic Partial Differential Equations

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In this presentation, we study the numerical approximation of a class of Backward Stochastic Differential Equations (BSDEs) in an infinite horizon setting that provide a probabilistic representation for semi-linear elliptic Partial Differential Equations. In particular, we are also able to treat some ergodic BSDEs that are related to elliptic PDEs or ergodic type. In order to build our numerical scheme, we put forward a new representation of the PDE solution by using a classical probabilistic representation of the gradient. Then, based on this representation, we propose a fully implementable numerical scheme using a Picard iteration procedure, a grid space discretization and a Monte-Carlo approximation. We obtain an upper bound for the numerical error and we also provide some numerical experiments that show the efficiency of this approach for small dimensions. Some numerical experiments also show that it is possible to efficiently handle larger dimensions by replacing grid-based spatial discretization with neural networks. This presentation is based on [1] for the non ergodic framework and [2] for results concerning the ergodic case.

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Mon, July 28 15:30-17:30 Track J

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As is known, the nonlinear Boltzmann equation describes the behavior of rarefied gas much better than the linear Kac's [1] model. That is why we can expect that application of the nonlinear spatially homogenous Boltzmann equation to the Harlow's "particles-in-cell" model [2] allows us to do a computation, which gives a more exact approximation of the solution. Among the statistical methods [3], which use Monte Carlo directly for modeling the flow of rarefied gas, the most efficient one is the statistical method of direct modeling the nonstationary flow. In the known "particle-in-cell" method, the simulations divide into

two steps. Monte Carlo method is used both for the numerical simulation of collisions of the particles in cells (the first step), as well as for the collision-free moving of particles (the second step). In this work we propose another computational scheme, which directly uses the non- linear spatially homogenous Boltzmann equation for the numerical realization of the first step in the "particles-in-cell" model of Belotserkovski-Yanitskii [3]. Proposed a new approach of constructing unbiased estimators will give relatively small variance. For this aim we construct a branching Markov process [4] and on its trajectory we propose various" conjugated" computational schemes for calculating an unbiased estimator of the given functional. It should be noted nowadays in this area became popular adjoint direct simulation Monte Carlo method to a general collision kernel [5]. The results of our computations show that they are similar with known Belotserkovski-Yanitskii solutions of the Boltzmann equation. We note that in the interval, where the Boltzmann equations" work" (intermediate interval), the "particle-in-cell" statistical model approximates the spatially heterogeneous Boltzmann equation better.

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Mon, July 28 15:30-17:30 Track J

A New Approach for Unbiased Estimation of Parameters of Partially Observed Diffusions

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In this talk, we consider the estimation of static parameters for a partially observed diffusion process with discrete-time observations over a fixed time interval. We develop particle filtering methods using time-discretization schemes, and we employ particle Markov chain Monte

Carlo methods to estimate the smoothing distribution. In particular, we use backward sampling to address the issue of sample degeneracy. We use the score function and stochastic gradient ascent methods to maximize the likelihood of the observations. Parameter estimation in the diffusion term is possible by introducing bridge processes and the corresponding bridge-guiding proposals. To achieve an unbiasedness, we adopt the Rhee and Glynn approach [1], in which the sources of bias are the number of stochastic gradient ascent steps and the time-discretization. Finally, we display numerically the method applying it to two systems.

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Mon, July 28 15:30-17:30 Track J

High-order adaptive methods for exit times of diffusion processes and reflected diffusions

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The Feynman–Kac formula connects domain-exit and boundary-reflection properties of stochastic differential equations (SDEs) and parabolic partial differential equations. The SDE viewpoint is particularly interesting for numerical methods, as it can be used with Monte Carlo methods to overcome the curse of dimensionality when solving high-dimensional PDE. This however hinges on having an efficient numerical method for simulating the exit times of SDEs. Since exit times of diffusion processes are very sensitive to perturbations in initial conditions, it is challenging to construct such numerical methods.

This talk presents a high-order method with adaptive time-stepping for strong approximations of exit times. The method employs a high-order Itô–Taylor scheme for simulating SDE paths and carefully decreases the step size in the numerical integration as the diffusion process approaches the domain's boundary. These techniques complement each other well: adaptive time-stepping improves the accuracy of the exit time by reducing the overshoot out of the domain, and high-order schemes improve the state approximation of the diffusion process, which is useful feedback to control the step size. We will also consider an ongoing extension of the numerical method to reflected diffusions.

Thu, July 31 10:30-12:30 Track E

Learning cooling strategies in simulated annealing through binary interactions

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Global optimization is amongst the hardest to solve problems. This is because finding the global minimum can usually only be guaranteed to be found in infinite time. Therefore one usually relies on meta-heuristic algorithms to guide the search and improve chances of successfully identifying the minimum. One particular family of algorithms is simulated annealing (SA). This family of algorithms is inspired by real-world metallurgy and is based on the Metropolis-Hastings algorithm. It works by randomly sampling N particles on the search space, each with a given temperature T. The movement of these particles is analogous to a Brownian random walk with step size proportional to temperature. The temperature is gradually cooled down over the course of the simulation according to some predefined schedule. Due to the Metropolis-Hastings-like acceptance-rejection rule, these particles can jump out of local minima and are expected to move towards the lowest energy state, i.e., the global minimum. It is the design of these cooling schedules for SA that we wish to improve. This is because they directly impact the efficiency of the optimization tool. Typically cooling schedules are inverse logarithmic or geometric decays in time. Here, we consider a collective SA dynamic where particles *interact* to learn the optimal temperature cooling strategy. This is inspired by the well-known particle-swapping technique known as parallel tempering (PT). To this aim we introduce a Boltzmann-type description where particles (partially) exchange their temperatures, therefore slowly cooling down the overall mean temperature. In order to simulate the dynamic we use a direct simulation Monte Carlo (DSMC) algorithm known as Nanbu-Babovsky. We show on various test functions (Ackley, Rastrigin, etc.) that this novel approach outperforms the standard SA with logarithmic and geometric annealing schedules.

Thu, July 31 10:30-12:30 Track E

Accuracy of Discretely Sampled Stochastic Policies in Continuous-Time Reinforcement Learning

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How to execute a stochastic policy in continuous-time environments is crucial for real-time operations and decision making. We show that, by sampling actions from a stochastic policy

at a fixed time grid and then executing a piecewise constant control process, the controlled state process converges to the corresponding aggregated dynamics in the weak sense as the grid size shrinks to zero and obtain the convergence rate. Specifically, under sufficiently regular conditions on the coefficients, the optimal convergence rate of $O(|\mathscr{G}|)$ is achieved with respect to the time grid $\mathscr{G}$. For less regular coefficients, a convergence rate is established that varies according to the degree of regularity of the coefficients. Additionally, we also derive large deviation bounds for the weak error. Beyond weak error convergence, strong convergence results are proved with a convergence order of $O(|\mathscr{G}|^{1/2})$ in cases where volatility is uncontrolled. Furthermore, we provide a counterexample to demonstrate that no strong convergence occurs when volatility is controlled. Based on these results, we analyze the bias and variance of the policy evaluation and policy gradient estimators in various algorithms for continuous-time reinforcement learning caused by discrete sampling.

Thu, July 31 10:30-12:30 Track E

Martingale deep neural networks for quasi-linear PDEs and stochastic optimal controls in 10,000 dimensions

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Coauthor(s): Shuixing Fang, Wenzhong Zhang, Tao Zhou

Abstract: In this talk, we will present a highly parallel and derivative-free martingale neural network method, based on the probability theory of Varadhan's martingale formulation of PDEs, to solve Hamilton-Jacobi-Bellman (HJB) equations arising from stochastic optimal control problems (SOCPs), as well as general quasilinear parabolic partial differential equations (PDEs). In both cases, the PDEs are reformulated into a martingale problem such that loss functions will not require the computation of the gradient or Hessian matrix of the PDE solution, and can be computed in parallel in both time and spatial domains. Moreover, the martingale conditions for the PDEs are enforced using a Galerkin method realized with adversarial learning techniques, eliminating the need for direct computation of the conditional expectations associated with the martingale property. For SOCPs, a derivative-free implementation of the maximum principle for optimal controls is also introduced. The numerical results demonstrate the effectiveness and efficiency of the proposed method, which is capable of solving HJB and quasilinear parabolic PDEs accurately and fast in dimensions as high as 10,000.

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Thu, July 31 10:30-12:30 Track E

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Minimizing a function with limited sample points is challenging when function evaluations are costly. We propose a fast interpolation-based approach using the Fast Fourier Transform (FFT) to estimate the minimum more efficiently. By interpolating from a sparse set of samples, our method achieves high accuracy with significantly fewer function evaluations. Preliminary results demonstrate its effectiveness for smooth periodic functions.

Fri, August 1 9:00–10:30 Track E

Delayed Acceptance Slice Sampling: A Two-Level method for Improved Efficiency in High-Dimensional Settings

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Coauthor(s): Bjoern Sprungk, Daniel Rudolf

Slice sampling is a Markov chain Monte Carlo (MCMC) method for drawing (approximately) random samples from a posterior distribution that is typically only known up to a normalizing constant. The method is based on sampling a new state on a slice, i.e., a level set of the target density function. Slice sampling is especially interesting because it is tuning-free and guarantees a move to a new state, which can result in a lower autocorrelation compared to other MCMC methods. However, finding such a new state can be computationally expensive due to frequent evaluations of the target density, especially in high-dimensional settings. To mitigate these costs, we introduce a delayed acceptance mechanism that incorporates an approximate target density for finding potential new states. We will demonstrate the effectiveness of our method through various numerical experiments and outline an extension of our two-level method into a multilevel framework.

Fri, August 1 9:00–10:30 Track E

Gradient-based MCMC in high dimensions

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Coauthor(s): Jakob Robnik, Uroš Seljak

Sampling from distributions over $\mathbb{R}^d$ for d larger than 10^4 arises as a computational challenge in many of the physical sciences, including particle physics [1], condensed matter physics [2], cosmology [3] and chemistry [4], as well as in Bayesian statistics and machine learning [5]. Commonly used gradient-based variants of Markov Chain Monte Carlo such as Hamiltonian Monte Carlo (HMC) [6] and in particular the No U-Turn Sampler [7], are designed for differentiable multivariate densities, but struggle in very high dimensions. We propose a general purpose approach to the gradient-based high dimensional regime, based on two insights. First, in high dimensional cases where limited asymptotic bias is acceptable, Markov Chain algorithms without Metropolis-Hastings (MH) adjustment are more statistically efficient; we provide theoretical and numerical evidence for this claim and show how to choose a step size to limit the incurred bias to an acceptable level. Second, in the case that MH adjustment is required, we show that a particular 4th order integrator [8] drastically improves the statistical efficiency of HMC and related algorithms in high dimensions.

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Fri, August 1 9:00–10:30 Track E

Parallel Affine Transformation Tuning: Drastically Improving the Effectiveness of Slice Sampling

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The performance of MCMC samplers tends to depend on various properties of the target distribution, such as its covariance structure, the location of its probability mass, and its tail behavior. We propose *parallel affine transformation tuning* (PATT) [1], a methodological framework that relies on bijective affine transformations, a latent space construction, the adaptive MCMC principle, and interacting parallel chains, and acts as an intermediate layer between the target distribution and an MCMC method applied to it. By transforming a challenging target into a simpler one, PATT can harness the full potential of the underlying MCMC method.

According to our numerical experiments, PATT is particularly effective in its combinations with *elliptical slice sampling* (ESS) [2] and *Gibbsian polar slice sampling* (GPSS) [3]. For targets that are sufficiently well-behaved (e.g. posteriors in Bayesian logistic regression), these combinations produce samples of (empirically) dimension-independent quality at remarkably low computational cost, with PATT-ESS performing best for light-tailed targets and PATT-GPSS being the superior choice for heavy-tailed ones.

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Fri, August 1 9:00–10:30 Track E

Low-Rank Thinning

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Coauthor(s): Albert Gong, Abhishek Shetty, Raaz Dwivedi, Lester Mackey

The goal in thinning is to summarize a dataset using a small set of representative points. Remarkably, sub-Gaussian thinning algorithms like Kernel Halving and Compress can match the quality of uniform subsampling while substantially reducing the number of summary points. However, existing guarantees cover only a restricted range of distributions and kernel-based quality measures and suffer from pessimistic dimension dependence. To address these deficiencies, we introduce a new low-rank analysis of sub-Gaussian thinning that applies to any distribution and any kernel, guaranteeing high-quality compression whenever the kernel or data matrix is approximately low-rank. To demonstrate the broad applicability of the techniques, we design practical sub-Gaussian thinning approaches that improve upon the best known guarantees for approximating attention in transformers, accelerating stochastic gradient training through reordering, and distinguishing distributions in near-linear time.

Wed, July 30 10:30–12:30 Track D

Combining quasi-Monte Carlo with Stochastic Optimal Control for Trajectory Optimization of Autonomous Vehicles in Mine Counter Measure Simulations

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Coauthor(s): Filip Van Utterbeeck, Ben Lauwens

Modelling and simulating mine countermeasures (MCM) search missions performed by autonomous vehicles is a challenging endeavour. The goal of these simulations typically consists of calculating trajectories for autonomous vehicles in a designated zone such that the coverage (residual risk) of the zone is below a certain user defined threshold. We have chosen to model and implement the MCM problem as a stochastic optimal control problem, see [1]. Mathematically, the MCM problem is defined as minimizing the total mission time needed to survey a designated zone Ω for a given residual risk of not detecting sea mines in the user-chosen square domain, i.e.,

$$\min T_f, \tag{2.4}$$

subjected to

$$\mathbb{E}[q\,(T_F)] := \int_{\Omega} \mathrm{e}^{-\int_0^{T_F} \gamma(\boldsymbol{x}(\tau),\boldsymbol{\omega})\,d\,\tau} \phi\,(\boldsymbol{\omega})\,d\,\boldsymbol{\omega} \leq \text{Residual Risk}. \tag{2.5}$$

The output of our stochastic optimal control implementation consists of an optimal trajectory in the square domain for the autonomous vehicle. As shown in Eq. (2.5), the residual risk is mathematically represented as an expected value integral. In [2], we presented a novel relaxation strategy for the computation of the residual MCM risk, used in our stochastic optimal control formulation. This novel relaxation strategy ensures that the residual risk obtained at the end of the optimisation run is below the maximally allowed user requested residual risk. This was however not the case with our initial 'naive' implementation of the MCM problem. Our proposed relaxation strategy ensures that the user requested risk is satisfied by sequentially solving the stochastic optimal control problem with an ever increasing size of the domain. We combine this strategy with a quasi-Monte Carlo sampling scheme based on a Rank-1 Lattice rule for the computation of the expected value integral. We observe a speedup up to a factor two in terms of total computational cost in favour of quasi-Monte Carlo when compared to standard Monte Carlo.

[1] Blondeel, P., Van Utterbeeck, F., Lauwens, B. (2024). Modeling sand ripples in mine countermeasure simulations by means of stochastic optimal control. In: The 19th European Congress on Computational Methods in Applied Sciences and Engineering, ECCOMAS, Lisbon, Portugal (2024).

[2] Blondeel, P., Van Utterbeeck, F., Lauwens, B. (2025). Application of quasi-Monte Carlo in Mine Countermeasure Simulations with a Stochastic Optimal Control Framework, *arXiv preprint*

Wed, July 30 10:30–12:30 Track D

A Monte Carlo Approach to Designing a Novel Sample Holder for Enhanced UV-Vis Spectroscopy

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Coauthor(s): A. Agugliaro, S. Albergo, R. De Angelis, I. Di Bari, A. Sciuto, A. Tricomi

UV-Vis spectroscopy is one of the most widely used techniques for identifying and quantifying substances in water and other solvents due to its speed and reliability. Its applications span diverse scientific fields, including chemistry, biochemistry, and medicine, as well as industrial sectors such as the pharmaceutical and food industries. Moreover, it plays a crucial role in environmental monitoring, particularly in assessing water quality. While alternative methods such as Raman and Ring Down spectroscopy have emerged, the core design of UV-Vis spectrometers has remained largely unchanged since their inception. Typically, these instruments employ a light source, a monochromator, a standard 1 cm cuvette as the sample holder, and one or more photosensors.

In this work, we present a novel approach that leverages Monte Carlo simulation to optimize the design of the sample holder for enhanced UV-Vis spectroscopy. In particular, our

setup adopts a pulsed light source and a Silicon Photomultiplier (SiPM) with single-photon counting capability. Using the optical transport package available in the Geant4 toolkit, we characterized and optimized the new design. The innovative holder, crafted in PTFE for its high UV reflectivity, resembles an integrating sphere, which increases the photon path length in the solution and thereby enhances absorbance in the presence of absorbing substances. We also present a comparison between experimental data and Monte Carlo predictions for validation. With this new sample holder, the spectrophotometer exhibits enhanced detection sensitivity, especially at low concentrations.

Wed, July 30 10:30–12:30 Track D

ARCANE Reweighting: A technique to tackle the sign problem in the simulation of collider events in high energy physics

Prasanth Shyamsundar
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Negatively weighted events, which appear in the Monte Carlo (MC) simulation of particle collisions, significantly increase the computational resource requirements of current and future collider experiments in high energy physics. This work introduces an MC technique called ARCANE reweighting for reducing or eliminating negatively weighted events. The technique works by redistributing (via an additive reweighting) the contributions of different pathways within the simulator that lead to the same final event. The technique is exact and does not introduce any biases in the distributions of physical observables. ARCANE reweighting can be thought of as a variant of the parametrized control variates technique, with the added nuance that redistribution is performed using a deferred additive reweighting. The technique is demonstrated for the simulation of a specific collision process, namely $e^+e^- \longrightarrow q\bar{q} + 1\,jet$. The technique can be extended to several other collision processes of interest as well. This talk is based on the Refs [1] and [2].

[1] Shyamsundar, Prasanth (2025). *ARCANE Reweighting: A Monte Carlo Technique to Tackle the Negative Weights Problem in Collider Event Generation.* arXiv:2502.08052 [hep-ph].

[2] Shyamsundar, Prasanth (2025). *A Demonstration of ARCANE Reweighting: Reducing the Sign Problem in the MC@NLO Generation of $e^+e^- \longrightarrow q\bar{q} + 1\,jet$ Events.* arXiv:2502.08052 [hep-ph].

Wed, July 30 10:30–12:30 Track D

Multifidelity and Surrogate Modeling Approaches for Uncertainty Quantification in Ice Sheet Simulations

Nicole Aretz
Oden Institute for Computational Engineering and Sciencess, University of Texas at Austin
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Coauthor(s): Max Gunzburger, Mathieu Morlighem, Karen Willcox

Our work [1] uses multifidelity and surrogate modeling to achieve computationally tractable uncertainty quantification (UQ) for large-scale ice sheet simulations. UQ is of utmost importance to enable judicious policy decisions combating climate change. However, high-fidelity ice sheet models are typically too expensive computationally to permit Monte Carlo sampling. To reduce the computational cost while achieving the same target accuracy, we use multifidelity estimators to shift the computational burden onto less expensive surrogate models derived from coarser discretizations and approximated physics. In this talk, we compare three estimators — Multifidelity [2] and Multilevel [3] Monte Carlo, and the Best Linear Unbiased Estimator [4] — and present results for the expected ice mass loss of the Greenland ice sheet.

[1] Aretz, N., Gunzburger, M., Morlighem, M., & Willcox, K. (2025). Multifidelity uncertainty quantification for ice sheet simulations. Computational Geosciences, 29(1), 1-22.

[2] Peherstorfer, B., Willcox, K., & Gunzburger, M. (2016). Optimal model management for multifidelity Monte Carlo estimation. SIAM Journal on Scientific Computing, 38(5), A3163-A3194.

[3] Giles, M. B. (2015). Multilevel monte carlo methods. Acta numerica, 24, 259-328.

[4] Schaden, D., & Ullmann, E. (2020). On multilevel best linear unbiased estimators. SIAM/ASA Journal on Uncertainty Quantification, 8(2), 601-635.

Wed, July 30 14:00–16:00 Track I

Empirical Statistical Comparative Analysis of SNP Heritability Estimators and Gradient Boosting Machines (GBM) Using Genetic Data from the UK Biobank

Kazeem Adeleke[*1]
University of the West of England, UK
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Coauthor(s): Peter Ogunyinka[2], Emmanuel Ologunleko[3] and Dawud Agunbiade[4]

This study addresses the methodological challenges in estimating genetic heritability by

comparing traditional statistical approaches with advanced machine learning techniques. We evaluated three distinct methods: sibling regression, LD-score regression, and Gradient Boosting Machines (GBMs), using both simulated datasets and real-world data from the UK Biobank. Our methodology involved generating simulated genotypes following Mendelian inheritance patterns and creating corresponding phenotypes incorporating family-specific genetic effect sizes. We conducted Genome-Wide Association Studies (GWAS) on firstborn children from each family and performed comprehensive heritability analyses using all three methods. Results demonstrated that while sibling regression effectively captured within-family genetic similarities and LD-score regression accounted for population-wide linkage disequilibrium patterns, GBMs showed superior capability in predicting phenotypes by capturing complex genetic interactions. The integration of GBMs with traditional methods revealed enhanced predictive power and provided new insights into the genetic architecture of complex traits. Our findings emphasize the value of combining conventional statistical approaches with machine learning techniques for more robust heritability estimation in large-scale UK Biobank studies.

Wed, July 30 14:00–16:00 Track I

Cheap permutation testing

Carles Domingo-Enrich
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Coauthor(s): Raaz Dwivedi, Lester Mackey

Permutation tests are a popular choice for distinguishing distributions and testing independence, due to their exact, finite-sample control of false positives and their minimax optimality when paired with U-statistics. However, standard permutation tests are also expensive, requiring a test statistic to be computed hundreds or thousands of times to detect a separation between distributions. In this work, we offer a simple approach to accelerate testing: group your datapoints into bins and permute only those bins. For U and V-statistics, we prove that these cheap permutation tests have two remarkable properties. First, by storing appropriate sufficient statistics, a cheap test can be run in time comparable to evaluating a single test statistic. Second, cheap permutation power closely approximates standard permutation power. As a result, cheap tests inherit the exact false positive control and minimax optimality of standard permutation tests while running in a fraction of the time. We complement these findings with improved power guarantees for standard permutation testing and experiments demonstrating the benefits of cheap permutations over standard maximum mean discrepancy (MMD), Hilbert-Schmidt independence criterion (HSIC), random Fourier feature, Wilcoxon-Mann-Whitney, cross-MMD, and cross-HSIC tests.

Wed, July 30 14:00–16:00 Track I

Moving PCG beyond LCGs

Christopher Draper
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Coauthor(s): Michael Mascagni

PCG is a set of generators released by Melissa E. O'Neill in 2014 [1]. The original technical report outlined a number of lightweight scrambling techniques. Each scrambling technique offered some improvement to the quality of the linear congruential generators they were designed for. However the real strength of the scrambling techniques was that they could easily be combined in different combinations to offer much stronger improvements. The PCG technical report concludes with the creation of the PCG library, a popular PRNG library that implements a number of generators described in the technical report. Starting from the observation that the PCG work was narrowly focused on implementing their scrambling techniques for specific linear congruential generators, we explore the PCG scrambling techniques and their potential application for being applied to other PRNGs. We show the steps taken to generalize the PCG scrambling techniques to work with any arbitrary amount of bits and parameter values. Then test the PCG scrambling techniques across different linear congruential generators and then test the PCG scrambling techniques across a number of different PRNGs.

[1] Melissa E. O'Neill. 2014. PCG: A Family of Simple Fast Space-Efficient Statistically Good Algorithms for Random Number Generation. Technical Report HMC-CS-2014-0905. Harvey Mudd College, Claremont, CA.

Wed, July 30 14:00–16:00 Track I

Hybrid least squares for learning functions from highly noisy data

Yiming Xu
University of Kentucky
yiming.xu@uky.edu

Coauthor(s): Ben Adcock, Bernhard Hientzsch, Akil Narayan

Motivated by the request for efficient estimation of conditional expectations, we consider a least-squares function approximation problem with heavily polluted data. In such scenarios, existing methods based on the small noise assumption become suboptimal. We propose a hybrid approach that combines Christoffel sampling with optimal experimental design to address this issue. The proposed algorithm adheres to appropriate optimality criteria for both

sample points generation and function evaluation, leading to improved computational efficiency and sample complexity. We also extend the algorithm to convex-constrained settings with similar theoretical guarantees. Moreover, when the target function is defined as the expectation of a random field, we introduce adaptive random subspaces to approximate the target function and establish results concerning its approximation capacity. Our findings are corroborated through numerical studies on synthetic data and a more challenging stochastic simulation problem in computational finance.

Special Sessions

Stochastic Computation and Complexity, Part I: SDEs, Stochastic Optimization and Neural Networks

Organizer:

Thomas Müller-Gronbach
University of Passau
Thomas.Mueller-Gronbach@uni-passau.de

Session Description:
The session is devoted to algorithms and complexity for

- quadrature and strong approximation of SDEs and SPDEs, in particular under non-standard assumptions,
- high and infinite dimensional integration and approximation, and
- stochastic optimization and neural networks,

including connections to functional analysis and stochastic analysis.

Monday, August 19, 2024 – Morning, 10:30 – 12:30, STC 0020

Daniel Rudolf
Almost Sure Convergence Rates of Adaptive Increasingly Rare Markov Chain Monte Carlo p. **??**

Marcin Wnuk
Approximation of Vectors Using Adaptive Randomized Information p. **??**

Klaus Ritter
Upper and Lower Bounds for Pathwise Approximation of Scalar SDEs With Reflection p. **??**

Optimization Under Uncertainty

Organizers:

Philipp A. Guth
RICAM, Austrian Academy of Sciences
philipp.guth@ricam.oeaw.ac.at

Vesa Kaarnioja
University of Potsdam
vesa.kaarnioja@iki.fi

Claudia Schillings
Free University of Berlin
c.schillings@fu-berlin.de

Session Description:
Large-scale optimization problems based on partial differential equation models typically involve a number of uncertainties: for example, the material parameters, domain shape or sensor locations used to collect the measurements may not be perfectly known. The quantification of these uncertainties leads to challenging high-dimensional integration problems, which can be tackled efficiently using, e.g., multilevel Monte Carlo or quasi-Monte Carlo methods. The intersection of optimization and uncertainty quantification is an actively developing field of research, and this session aims to cover some recent advances in the computational and theoretical treatment of these topics.

Monday, August 19, 2024 – Morning, 10:30 – 12:30, STC 0040

Philipp Guth
Quasi-Monte Carlo Methods for Optimal Feedback Control Problems Under Uncertainty p. **??**

Helmut Harbrecht
Shape Optimization Under Constraints on the Probability of a Quadratic Functional to Exceed a Given Threshold p. **??**

Fabio Musco
Deep Learning Methods for Stochastic Galerkin Approximations of Random Elliptic PDEs p. **??**

Arved Bartuska
Randomized Quasi-Monte Carlo for Nested Integration p. **??**

Efficient Bayesian Surrogate Modeling, Part I

Organizers:

Aleksei Sorokin
Illinois Institute of Technology
asorokin@hawk.iit.edu

Pieterjan Robbe
Sandia National Laboratories
pmrobbe@sandia.gov

Session Description:
Common tasks in stochastic modeling include model calibration and sensitivity analysis. These tasks typically require many model evaluations, which can be prohibitively expensive in case model evaluations are costly. This has motivated the development of surrogate models, which are fit offline on a limited budget and then enable rapid online evaluations for predictive purposes. An important decision is where to evaluate the model in order to maximize information captured by the surrogate. While Monte Carlo points are a conventional choice, their independent nature often leads to sampling in locations of little value to the surrogate. In contrast, dependent structures, such as quasi-random (low discrepancy) points or Bayesian optimal experimental designs, have proven to produce more reliable surrogate models. This session will discuss some of the recent developments in these sampling techniques, and will bring together researchers from both communities to explore collaborations.

Monday, August 19, 2024 – Morning, 10:30 – 12:30, STC 0050

Pieterjan Robbe
Efficient Surrogate Construction for Response Surfaces With Steep Gradients p. **??**

Michael McCourt
Constraint Active Search as an Alternative to Multiobjective Optimization p. **??**

John Miller
Diverse Expected Improvement (DEI): Diverse Optimization of Expensive Black-Box Simulators for Internal Combustion Engine Control p. **??**

Stochastic Computation and Complexity, Part II: Approximation of SDEs Under Non-Standard Assumptions

Organizer:

Stefan Heinrich
RPTU Kaiserslautern-Landau
heinrich@informatik.uni-kl.de

Session Description:
The session is devoted to algorithms and complexity for

- quadrature and strong approximation of SDEs and SPDEs, in particular under non-standard assumptions,
- high and infinite dimensional integration and approximation, and
- stochastic optimization and neural networks,

including connections to functional analysis and stochastic analysis.

Monday, August 19, 2024 – Afternoon, 15:30 – 17:30, STC 0020

Christopher Rauhögger
Milstein-Type Methods for Strong Approximation of Systems of SDEs With a Discontinuous Drift Coefficient p. **??**

Łukasz Stepien
On Efficient Approximation of SDEs Driven by Countably Dimensional Wiener Process p. **??**

Simon Ellinger
On Optimal Error Rates for Strong Approximation of SDEs With a Hölder-Continuous Drift Coefficient p. **??**

Efficient Bayesian Surrogate Modeling, Part II

Organizers:

Aleksei Sorokin
Illinois Institute of Technology
asorokin@hawk.iit.edu

Pieterjan Robbe
Sandia National Laboratories
pmrobbe@sandia.gov

Session Description:
Common tasks in stochastic modeling include model calibration and sensitivity analysis. These tasks typically require many model evaluations, which can be prohibitively expensive in case model evaluations are costly. This has motivated the development of surrogate models, which are fit offline on a limited budget and then enable rapid online evaluations for predictive purposes. An important decision is where to evaluate the model in order to maximize information captured by the surrogate. While Monte Carlo points are a conventional choice, their independent nature often leads to sampling in locations of little value to the surrogate. In contrast, dependent structures, such as quasi-random (low discrepancy) points or Bayesian optimal experimental designs, have proven to produce more reliable surrogate models. This session will discuss some of the recent developments in these sampling techniques, and will bring together researchers from both communities to explore collaborations.

Monday, August 19, 2024 – Afternoon, 15:30 – 17:30, STC 0050

Aleksei Sorokin
Fast Gaussian Process Regression for Smooth Functions Using Lattice and Digital Sequences With Matching Kernels p. **??**

Vishwas Rao
Rare Events and Their Optimization p. **??**

Xun Huan
Bayesian Optimal Experimental Design for Surrogate Model Training p. **??**

Variance Reduction Techniques for Rare Events

Organizers:

Nadhir Ben Rached
University of Leeds
n.benrached@leeds.ac.uk

Raúl Tempone
RWTH Aachen University and KAUST
tempone@uq.rwth-aachen.de

Shyam Mohan Subbiah Pillai
RWTH Aachen University
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Session Description:
Rare events are events with small probabilities, but their occurrences are critical in many real-life applications. The problem of estimating rare event probabilities is encountered in various engineering applications (finance, wireless communications, system reliability, Biology, etc.). Naive Monte Carlo simulations are, in this case, substantially expensive. This session focuses on methods belonging to the class of variance reduction techniques. These alternative methods deliver, when appropriately used, accurate estimates with a substantial amount of variance reduction compared to the naive Monte Carlo estimator.

Monday, August 19, 2024 – Afternoon, 15:30 – 17:30, STC 0060

Eya Ben Amar
Importance Sampling Methods With Stochastic Differential Equations for the Estimation of the Right Tail of the CCDF of the Fade Duration p. **??**

Shyam Mohan Subbiah Pillai
Importance Sampling via Stochastic Optimal Control for Rare Events Associated With McKean-Vlasov Equation p. **??**

Romain Espoeys
Multilevel Reliability Analysis: Application to a Flood Risk Estimation p. **??**

Stochastic Computation and Complexity, Part III: Approximation of SDEs Under Non-Standard Assumptions

Organizer:

Thomas Müller-Gronbach
University of Passau
Thomas.Mueller-Gronbach@uni-passau.de

Session Description:
The session is devoted to algorithms and complexity for

- quadrature and strong approximation of SDEs and SPDEs, in particular under non-standard assumptions,
- high and infinite dimensional integration and approximation, and
- stochastic optimization and neural networks,

including connections to functional analysis and stochastic analysis.

Tuesday, August 20, 2024 – Morning, 10:30 – 12:30, STC 0020

Stefan Heinrich
Integration and Approximation of Functions by Monte Carlo and Quantum Methods p. **??**

Kateryna Pozharska
Sampling Recovery and Sharp Norm Estimates of Projection Operators p. **??**

Nicolas Nagel
The L2-Discrepancy of Latin Hypercubes p. **??**

Efficient Methods for Uncertainty Quantification in Differential Equations, Part I

Organizers:

Anastasia Istratuca
University of Edinburgh, Heriot-Watt University
a.istratuca@sms.ed.ac.uk

Aretha Teckentrup
University of Edinburgh
a.teckentrup@ed.ac.uk

Session Description:
One of the most common approaches to modelling physical phenomena consists of ordinary and partial differential equations, which allow for computer simulations through the use of modern numerical solvers. These models encompass parameters that often have to be measured or inferred from data. To account for error measurements and scarce availability of the data, we express our uncertainty about the parameters by associating, for example, a probability distribution to them. This mini-symposium focuses on recent advances in algorithms for quantifying the uncertainty in such models.

Tuesday, August 20, 2024 – Morning, 10:30 – 12:30, STC 0040

Sebastian Krumscheid
Nonparametric Inference for Diffusion Processes p. **??**

Elliot Addy
History Matching and Gaussian Process Emulation in High Dimensions p. **??**

Weiwen Mo
A Universal Lattice-Based Algorithm for Multivariate Function Approximation in Uncertainty Quantification p. **??**

Vesa Kaarnioja
Revisiting High-Dimensional Kernel Approximation of Parametric PDEs Over Lattice Point Sets p. **??**

Recent Advances in QMC Methods for Computational Finance and Financial Risk Management

Organizers:

Chiheb Ben Hammouda
Utrecht University
c.benhammouda@uu.nl

Raúl Tempone
RWTH Aachen University, King Abdullah University of Science and Technology
rtempone@gmail.com

Session Description:
The session is about recent numerical and theoretical advances in quasi-Monte Carlo (QMC) methods to address different challenges in computational finance and Risk management. Challenges range from pricing high-dimensional financial derivatives, computing sensitivities, and efficiently estimating nested expectations arising in financial risk estimation.

Tuesday, August 20, 2024 – Morning, 10:30 – 12:30, STC 0050

Efficient Methods for Uncertainty Quantification in Differential Equations, Part II

Organizers:

Anastasia Istratuca
University of Edinburgh, Heriot-Watt University
a.istratuca@sms.ed.ac.uk

Aretha Teckentrup
University of Edinburgh
a.teckentrup@ed.ac.uk

Session Description:
One of the most common approaches to modelling physical phenomena consists of ordinary and partial differential equations, which allow for computer simulations through the use of modern numerical solvers. These models encompass parameters that often have to be measured or inferred from data. To account for error measurements and scarce availability of the data, we express our uncertainty about the parameters by associating, for example, a probability distribution to them. This mini-symposium focuses on recent advances in algorithms for quantifying the uncertainty in such models.

Tuesday, August 20, 2024 – Afternoon, 15:30 – 17:30, STC 0040

Learning to Solve Related Integrals

Organizer:

Chris. J. Oates
Newcastle University, UK
chris.oates@ncl.ac.uk

Session Description:
The standard perspective on numerical analysis deals with solving individual numerical tasks, but in practice the experience gained from using numerical methods to solve related problems provides valuable insight into their performance, which can shape how and when numerical methods are used. Developments at the intersection of probability, statistics, and numerical analysis seek to leverage experience to improve performance on subsequent numerical tasks as they are encountered. This session will shine a light on emerging methodology for the solution of related integration problems, arising in areas of research that include sensitivity analysis, computational finance, the solution of partial differential equations, decision-making under uncertainty, and diffusion-based generative modelling. François-Xavier Briol from University College London will present a probabilistic approach to estimating related conditional expectations, which operates by sharing statistical information regarding the integrand. Jon Cockayne from the University of Southampton will present a novel statistical approach to solving related linear systems of equations, such as occur when integrating a partial differential equation that is parameter-dependent. Zheyang Shen from Newcastle University will present a novel perspective on diffusion-based generative modelling, which casts the problem of generating realistic image data as the estimation of related kernel mean embeddings in a reproducing kernel Hilbert space framework.

Tuesday, August 20, 2024 – Afternoon, 15:30 – 17:30, STC 0050

Francois-Xavier Briol
Estimating Parametric Expectations Through Bayesian Quadrature p. **??**

Jon Cockayne
Learning to Solve Related Linear Systems p. **??**

Zheyang Shen
Demystifying Diffusion Models via Their Markov Semigroups p. **??**

Function Recovery and Discretization Problems, Part I

Organizers:

David Krieg
Institute of Analysis, Johannes Kepler University Linz, Austria
david.krieg@jku.at

Kateryna Pozharska
Institute of Mathematics of NAS of Ukraine, Kyiv, Ukraine;
Faculty of Mathematics, Chemnitz University of Technology, Germany
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Session Description:
In this session, we would like to bring together experts who contributed to the theory of function recovery and related problems. Recently, there has been much progress in understanding the power of different types of information (function values vs. linear measurements, optimal vs. random) as well as different classes of algorithms (linear vs. nonlinear, random vs. deterministic, adaptive vs. nonadaptive), but also with regard to the error analysis for specific recovery schemes. The session is concerned with these new developments, which also include the impact of a large dimension, discretization in function spaces and modern methods in data science.

Wednesday, August 21, 2024 – Morning, 10:30 – 12:30, STC 0020

Testing and Analysis of Pseudorandom Number Generators

Organizers:

Emil Løvbak
Karlsruhe Institute of Technology
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Michael Mascagni
Florida State University
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Session Description:
Pseudorandom number generators are a core part of scientific computing, lying at the foundation of Monte Carlo methods. Over the history of the field, the quality of such generators has consistently been improved to produce streams of numbers that are hard to distinguish from truly random numbers. There are two approaches to quantify the randomness of a given generator. On the one hand, one can use mathematical techniques to determine the theoretical properties of the generator such as period length, uniformity, and sequence correlation. On the other hand, one can apply statistical benchmarks to empirically test the streams produced by a generator. This minisymposium aims to bring together researchers working on the design and testing of practical random number generators to exchange ideas on how to make use of these two complementary approaches in their evaluation.

Wednesday, August 21, 2024 – Morning, 10:30 – 12:30, STC 0050

Function Recovery and Discretization Problems, Part II

Organizers:

David Krieg
Institute of Analysis, Johannes Kepler University Linz, Austria
david.krieg@jku.at

Kateryna Pozharska
Institute of Mathematics of NAS of Ukraine, Kyiv, Ukraine;
Faculty of Mathematics, Chemnitz University of Technology, Germany
pozharska.k@gmail.com

Session Description:
In this session, we would like to bring together experts who contributed to the theory of function recovery and related problems. Recently, there has been much progress in understanding the power of different types of information (function values vs. linear measurements, optimal vs. random) as well as different classes of algorithms (linear vs. nonlinear, random vs. deterministic, adaptive vs. nonadaptive), but also with regard to the error analysis for specific recovery schemes. The session is concerned with these new developments, which also include the impact of a large dimension, discretization in function spaces and modern methods in data science.

Wednesday, August 21, 2024 – Afternoon, 15:30 – 17:30, STC 0020

Universality in QMC and Related Algorithms

Organizer:

Peter Kritzer
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peter.kritzer@oeaw.ac.at

Session Description:
In the literature on QMC and related methods, it is often the case that one can tailor an algorithm to a specific problem, usually depending on a certain (fixed) choice of problem parameters such as smoothness parameters or coordinate weights. This may have the advantage that one obtains an excellent algorithm for this particular problem, but the obvious downside is that it is not clear whether the same algorithm could be applied in other settings, e.g., when some of the parameters change. There have been recent attempts to make QMC and related algorithms more universal, and a number of interesting open questions remain. This special session brings together four speakers who have recently contributed to this aspect of multivariate algorithms.

Wednesday, August 21, 2024 – Afternoon, 15:30 – 17:30, STC 0040

Josef Dick
Explicit Constructions of Point Sets Whose Worst-Case Error in Certain Spaces Depends Polynomially on the Dimension p. **??**

Fred Hickernell
Quasi-Monte Carlo Kernel Density Estimation p. **??**

Kosuke Suzuki
A Universal Median Quasi-Monte Carlo Integration p. **??**

Laurence Wilkes
Using Kronecker Point Sets for Function Approximation in the Korobov Space p. **??**

Multilevel Methods for SDEs and SPDEs, Part I

Organizer:

Mike Giles
University of Oxford
mike.giles@maths.ox.ac.uk

Session Description:
Speakers in this session will present and analyse multilevel algorithms for an interesting variety of applications, including chaotic SDEs, stochastic PDEs and kinetic particle models.

Thursday, August 22, 2024 – Morning, 10:30 – 12:30, STC 0020

Recent Advances in Monte Carlo Methods for Forward and Inverse Problems for Stochastic Reaction Networks, Part I

Organizers:

Chiheb Ben Hammouda
Utrecht University
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Sophia Wiechert
RWTH Aachen University
wiechert@uq.rwth-aachen.de

Raúl Tempone
RWTH Aachen University
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Session Description:
The session is about recent advances related to Monte Carlo methods and variance/dimension reduction techniques for forward/inverse problems and sensitivity analysis for pure jump processes and stochastic reaction networks, with a particular focus on stochastic biological and chemical systems.

Thursday, August 22, 2024 – Morning, 10:30 – 12:30, STC 0040

Kernel Approximation and Cubature, Part I

Organizers:

Vesa Kaarnioja
University of Potsdam
vesa.kaarnioja@iki.fi

Ilja Klebanov
Free University of Berlin
klebanov@zedat.fu-berlin.de

Session Description:
Reproducing kernel Hilbert spaces (RKHSs) are very amenable to the development of efficient approximation and cubature methods. To this end, there has been a surge of interest in recent years regarding some of the advantages that kernel-based methods can offer in applications involving collocation over Monte Carlo or quasi-Monte Carlo point sets—some examples include, e.g., Gaussian process regression (kriging), Bayesian neural networks or uncertainty quantification for partial differential equations. This minisymposium showcases some recent theoretical and computational developments in the study of kernel-based approximation and cubature methods.

Thursday, August 22, 2024 – Morning, 10:30 – 12:30, STC 0050

Ian Sloan
High Dimensional Approximation -- Making Life Easy With Kernels p. **??**

Robert Gruhlke
Quasi-Monte Carlo Meets Kernel Cubature p. **??**

Chris Oates
Sampling With Stein Discrepancies p. **??**

Ilja Klebanov
Enhanced Lattice-Based Kernel Cubature Through Weight Optimization p. **??**

Multilevel Methods for SDEs and SPDEs, Part II

Organizer:

Mike Giles
University of Oxford
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Session Description:
Speakers in this session will present and analyse multilevel algorithms for an interesting variety of applications, including chaotic SDEs, stochastic PDEs and kinetic particle models.

Thursday, August 22, 2024 – Afternoon, 15:30 – 17:30, STC 0020

Recent Advances in Monte Carlo Methods for Forward and Inverse Problems for Stochastic Reaction Networks, Part II

Organizers:

Chiheb Ben Hammouda
Utrecht University
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Sophia Wiechert
RWTH Aachen University
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Raúl Tempone
RWTH Aachen University
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Session Description:
The session is about recent advances related to Monte Carlo methods and variance/dimension reduction techniques for forward/inverse problems and sensitivity analysis for pure jump processes and stochastic reaction networks, with a particular focus on stochastic biological and chemical systems.

Thursday, August 22, 2024 – Afternoon, 15:30 – 17:30, STC 0040

Kernel Approximation and Cubature, Part II

Organizers:

Vesa Kaarnioja
University of Potsdam
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Ilja Klebanov
Free University of Berlin
klebanov@zedat.fu-berlin.de

Session Description:
Reproducing kernel Hilbert spaces (RKHSs) are very amenable to the development of efficient approximation and cubature methods. To this end, there has been a surge of interest in recent years regarding some of the advantages that kernel-based methods can offer in applications involving collocation over Monte Carlo or quasi-Monte Carlo point sets—some examples include, e.g., Gaussian process regression (kriging), Bayesian neural networks or uncertainty quantification for partial differential equations. This minisymposium showcases some recent theoretical and computational developments in the study of kernel-based approximation and cubature methods.

Thursday, August 22, 2024 – Afternoon, 15:30 – 17:30, STC 0050

Dirk Nuyens
A Comparison of Lattice Based Kernel and Truncated Least Squares Approximations p. **??**

Abirami Srikumar
Approximating Distribution Functions in Uncertainty Quantification Using Quasi-Monte Carlo Methods p. **??**

Laura Bazahica
Quasi-Monte Carlo for Electrical Impedance Tomography p. **??**

André-Alexander Zepernick
Quasi-Monte Carlo Methods for PDEs on Randomly Moving Domains p. **??**

MCMC: Convergence and Robustness

Organizers:

Alex Shestopaloff
Queen Mary University of London
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Jun Yang
University of Copenhagen
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Session Description:
As Markov Chain Monte Carlo (MCMC) methods become more complex, a deeper understanding of their convergence and performance guarantees in realistic scenarios becomes an important aspect of using these methods in computational Bayesian statistics. This session aims to further this understanding by focusing on the convergence and robustness of complex MCMC samplers, covering recent work on topics such as convergence of hybrid Gibbs sampling [1], novel methods for evaluation of convergence rates using random number simulations [2] the study of convergence with Dirichlet forms [3] as well as techniques for making MCMC samplers more robust and a study of their corresponding convergence properties, such as [4].

[1] Qian Qin, Nianqiao Ju, Guanyang Wang (2023). Spectral gap bounds for reversible hybrid Gibbs chains. arXiv:2312.12782.

[2] Sabrina Sixta and Jeffrey S. Rosenthal (2023). Bounding and estimating MCMC convergence rates using common random number simulations. arXiv:2309.15735.

[3] Ning Ning (2022). Convergence of Dirichlet Forms for MCMC Optimal Scaling with General Target Distributions on Large Graphs. arXiv:2210:17042.

[4] Michael C.H. Choi (2020). Improved Metropolis-Hastings algorithms via landscape modifcation with applications to simulated annealing and the Curie-Weiss model. arXiv: 2011:09680.

Friday, August 23, 2024 – Morning, 10:30 – 12:30, STC 0020

Michael Choi
Geometric Unification of Central MCMC Algorithms via Rate Distortion Theory and Factorizability of Multivariate Markov Chains p. **??**

Federica Milinanni
A Large Deviation Principle for Metropolis-Hastings Sampling p. **??**

Ning Ning
On the Convergence of MCMCs With Quantum Speedup p. **??**

Cameron Bell
Adapting the Stereographic Bouncy Particle Sampler p. **??**

Continuous-Time Dynamics in Monte Carlo and Beyond

Organizers:

Neil Chada
Heriot-Watt University
n.chada@hw.ac.uk

Jonas Latz
University of Manchester
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Session Description:
Langevin Monte Carlo methods — such as MALA and ULA [3] — construct a Monte Carlo Markov chain by appropriately discretising certain stochastic differential equations. This has the fortunate effect that certain properties of the resulting MCMC algorithms can be derived by studying these SDEs rather than the arising discrete-time Markov chains. The idea of analysing an underlying continuous-time system to understand a discrete-time algorithm is much broader and shall be one focus of this minisymposium – with 'algorithm', we foremost want to focus on methods in computational statistics, but also look forward to optimisation methods, such as [2], data assimilation, diffusion models, and partial differential equation methods in data science. The second focus are Monte Carlo methods that are both posed and used in continuous time, such as piecewise-deterministic Markov processes (cf. [1]).

[1] Bierkens, Joris, Paul Fearnhead & Gareth Roberts (2019). *The Zig-Zag process and super-efficient sampling for Bayesian analysis of big data.* Ann. Statist. 47(3): 1288-1320.

[2] Li, Qianxiao , Cheng Tai & Weinan E (2019). *Stochastic Modified Equations and Dynamics of Stochastic Gradient Algorithms I: Mathematical Foundations.* J. Mach. Learn. Res. 20(40):1-47.

[3] Roberts, Gareth & Richard Tweedie (2002). *Exponential convergence of Langevin distributions and their discrete approximations.* Bernoulli 2(4): 341-363.

Friday, August 23, 2024 – Morning, 10:30 – 12:30, STC 0040

Function Spaces and Algorithms for High-Dimensional Problems

Organizers:

Michael Gnewuch
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Klaus Ritter
RPTU Kaiserslautern, Germany
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Session Description:
High- and infinite-dimensional problems pose serious challenges in numerical practice. An approach to surpass these obstacles is to identify common structural features of the underlying problems. These features are usually encoded in the specific function spaces that are considered in the analysis. In this special session we want to bring together researchers from analysis, approximation theory, and information-based complexity to discuss different types of function spaces and algorithmic approaches for high- and infinite-dimensional integration and approximation problems.

Friday, August 23, 2024 – Morning, 10:30 – 12:30, STC 0050

Michael Gnewuch
Function Space Embeddings for Non-Tensor Product Spaces and Application to High-Dimensional Approximation p. **??**

Laura Weidensager
ANOVA-Boosting for High-Dimensional Approximation p. **??**

Robin Rüßmann
Tractability Results for Integration on Gaussian Spaces p. **??**