GIP – Gesellschaft für Inverse Probleme e.V.

CRC 1456
MATHEMATICS OF EXPERIMENT

SFB 1294
Data Assimilation

Symposium on Inverse Problems

From experimental data to models and back

As part of
the newly established

Potsdam DA Days

University of Potsdam
Campus Griebnitzsee

Universität Potsdam

Invited Speakers:

September
19th-21st
2 0 2 2

Gilles Blanchard
Université Paris Saclay

Marc Bocquet
École des Ponts ParisTech

Cristina Butucea
ENSAE, IP Paris

Elizabeth Qian
California Institute of Technology

Tim Salditt
University of Göttingen

Georg Stadler
Courant Institute of Mathematical Sciences, NY University

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SYMPOSIUM ON INVERSE PROBLEMS

From experimental data to models and back

POTSDAM
DATA ASSIMILATION DAYS

September
19th – 21st
2022

Potsdam, Griebnitzsee

Funded and co-organized by

DFG Deutsche Forschungsgemeinschaft

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CONTENT

MESSAGE FROM THE SCIENTIFIC COMMITTEE

The scientific committee would like to thank Lydia Stopmann (Potsdam), Eva Hetzel and Norma Rahlfs-Rittmeier (Göttingen), and Jana Hilber (Chemnitz, GIP) for their great work in supporting the organization of this conference.

The symposium is both Annual Meeting of the GIP and kick off of the newly established Potsdam DA Days. In total, 61 abstracts have been submitted for a contribution at this symposium and have been reviewed by the scientific committee. The 3-day program with 102 registered participants includes plenary talk of 6 invited speakers, 30 oral presentations, and a poster session with 23 poster contributions.

Thank you all for coming to Potsdam and we are looking forward to three days full of exciting scientific discussions and exchanges.

Yours sincerely,

Melina Freitag, Thorsten Hohage, Axel Munk, Ronny Ramlau, Sebastian Reich, and Markus Reiß

PROGRAM

Monday, September 19, 2022		
09:00	*REGISTRATION & WELCOME*	
09:30	**Plenary Talk 1 | Lecture hall H03 & H04** (Chair: Sebastian Reich) **Current Challenges in Phase Retrieval and Tomographic Reconstruction: Inverse Problems at Work** Tim Salditt (University of Göttingen, Göttingen, DE)	
10:20	*COFFEE BREAK*	
	Session 1 | Lecture hall H03 ***PDE 1*** (Chair: Jan-F. Pietschmann)	**Session 2 | Lecture hall H04** ***Computational Approaches 1*** (Chair: Mihaela Pricop-Jeckstadt)
10:50	Reconstruction of Inclusions in Elastic Bodies Based on Experimental Data (Sarah Eberle, Frankfurt)	Challenges of dynamic data: joint reconstruction and motion estimation in MPI (Lena Zdun, Hamburg)
11:20	Quantitative elastic diffraction tomography (Bochra Mejri, Linz)	Multilevel Optimization for Inverse Problems (Simon Weissmann, Heidelberg)
11:50	On Recovering the Fractional Damping Operator in a Wave Equation from Time Trace Data (William Rundell, Texas)	An augmented Krylov subspace method for atmospheric tomography (Bernadett Stadler, Linz)
12:20	*LUNCH*	
14:00	**Plenary Talk 2 | Lecture hall H03 & H04** (Chair: Melina Freitag) **Balanced truncation for Bayesian inference** Elizabeth Qian (California Institute of Technology, Pasadena, US)	
14:50	*COFFEE BREAK*	

Monday, September 19, 2022		
	Session 3 | Lecture hall H03 ***Bayesian Methods 1*** (Chair: Simon Weissmann)	**Session 4 | Lecture hall H04** ***Machine Learning*** (Chair: Claudia Schillings)
15:20	Geodesic slice sampling on the sphere (Mareike Hasenpflug, Passau)	Multi-armed bandit problem with side observations (Tomáš Kocák, Potsdam)
15:50	Bayesian Structure Determination from Single Molecule X-Ray Diffraction (Steffen Schultze, Göttingen)	Sequential Learning (Karen Seidel, Potsdam)
16:20	Bayesian hypothesis testing in statistical inverse problems (Remo Kretschmann, Würzburg)	
16:50	*COFFEE BREAK*	
17:20	**Poster Lightning**	
17:50	*ICE BREAKER & POSTER SESSION*	

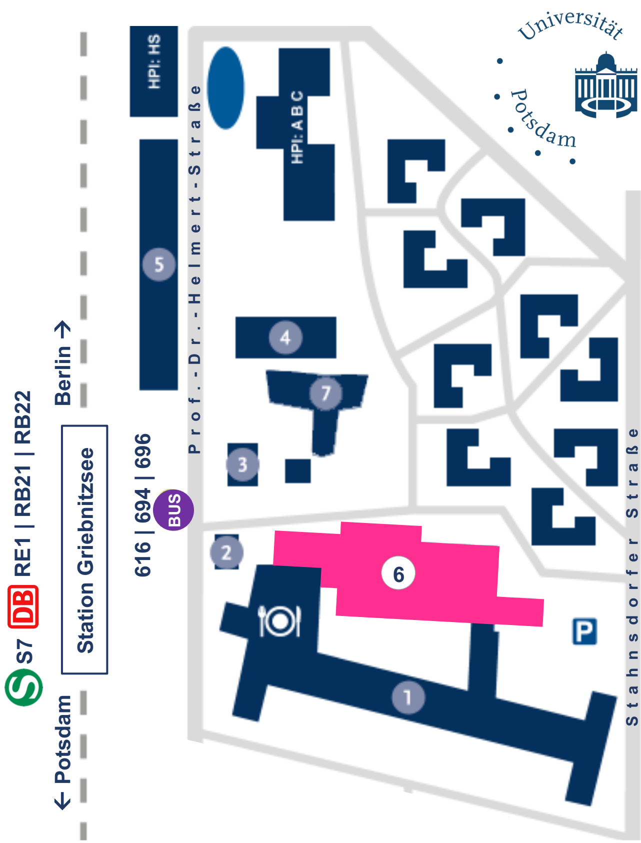
Tuesday, September 20, 2022		
09:00	**Plenary Talk 3 | Lecture hall H03 & H04** (Chair: Ronny Ramlau) **Bayesian online algorithms for learning data-driven models of chaotic dynamics** Marc Bocquet (CEREA, École des Ponts & EdF R&D, Île-de-France, FR)	
09:50	*COFFEE BREAK*	
10:20	**Plenary Talk 4 | Lecture hall H03 & H04** (Chair: Axel Munk) **Simultaneous adaptation for several criteria in inverse learning problems using an extended Lepskiĭ principle** (Gilles Blanchard, Université Paris, FR)	
	Session 5 | Lecture hall H03 ***Machine Learning and PDE*** (Chair: Han Cheng Lie)	**Session 6 | Lecture hall H04** ***Computational Approaches 2*** (Chair: Frank Werner)
11:20	Learning a regularized solution from infinitely many trial functions (Naomi Schneider, Siegen)	Subaperture-based Digital Aberratio Correction for OCT (Simon Hubmer, Linz)
11:50	Data driven gradient flows (Jan-F. Pietschmann, Chemnitz)	Numerical algorithms for a stochastic realization problem (Martin Hanke-Bourgeois, Mainz)
12:20	*GROUP PHOTO*	
12:30	*LUNCH*	
14:00	**Plenary Talk 5 | Lecture hall H03 & H04** (Chair: Markus Reiss) **Off-the-grid estimation of sparse mixtures** (Cristina Butucea, ENSAE, IP Paris, FR)	
14:50	*COFFEE BREAK*	

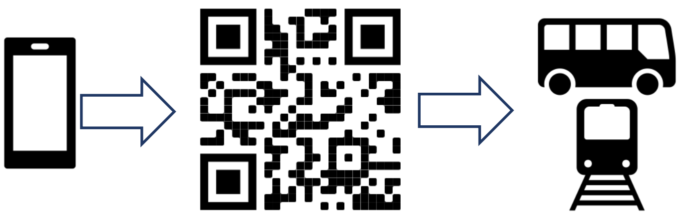
Tuesday, September 20, 2022		
	Session 7 | Lecture hall H03 ***Bayesian Approaches 2*** (Chair: Vladimir Spokoiny)	**Session 8 | Lecture hall H04** ***Regularization of Inverse Problems in PDEs*** (Chair: Tim Jahn)
15:20	Adaptive MCMC for doubly intractable distributions (Julian Hofstadler, Passau)	Weighted regularization for identifying sources from Cauchy boundary data (Bjøen F. Nielsen, Ås)
15:50	Overconfidence and randomisation in numerical Bayesian inverse problems (Han Cheng Lie, Potsdam)	Variational Source Condition for an Inverse Source Problem (Philipp Mickan, Göttingen)
16:20	Optimal rates of convergence for functional data analysis with indirect observations (Mihaela Pricop-Jeckstadt, Bucharest)	Ill-posedness of time-dependent inverse problems in Lebesgue-Bochner spaces (Thomas Schuster, Saarbrücken)
16:50	*COFFEE BREAK*	
17:20 – 18:20	**GIP Award for the best PhD thesis**	

Wednesday, September 21, 2022		
09:00	**Plenary Talk 6 | Lecture hall H03 & H04** (Chair: Thorsten Hohage) **Optimal design of experiments for Bayesian inverse problems governed by PDEs** (Georg Stadler, NY University, New York, US)	
09:50	*COFFEE BREAK*	
	Session 9 | Lecture hall H03 ***PDE 2*** (Chair: William Rundell)	**Session 10 | Lecture hall H04 Comput/Bay/PDE** (Chair: Martin Hanke-Bourgeois)
10:20	An Improved Adaptive Spectral Inversion for Inverse Problems (Yannik Gleichmann, Basel)	Solving a quantitative passive imaging problem in helioseismology by iterative holography: Inversions for solar differential rotation (Björn Müller, Göttingen)
10:50	Some inverse problems for wave equations with fractional derivative attenuation (Barbara Kaltenbacher, Klagenfurt)	Greedy sensor placement for Bayesian inverse problems via model order reduction (Nada Cvetkovic, Eindhoven)
11:20	Optical diffraction tomography with an object rotated into arbitrary (Michael Quellmalz, Berlin)	Optimal design of experimental conditions for a Bayesian inverse problem in photoacoustic imaging (Karina Koval, Heidelberg)
11:50	*COFFEE BREAK*	
	Session 11 | Lecture hall H03 ***Regularization*** (Chair: Simon Hubmer)	**Session 12 | Lecture hall H04** ***High Dimensional IP*** (Chair: Ralf Engbert)
12:20	Tikhonov Regularization - Low order convergence Rates for a discrepancy principle under low order source conditions in the oversmoothing case (Chantal Klinkhammer, Siegen)	Modeling Eye Movement: What DNNs And Biological Models Can Teach Each Other (Lisa Schwetlick, Potsdam)
12:50	Discretisation-adaptive regularization of statistical inverse (Tim Jahn, Bonn)	Sparse optimization methods for infinite-dimensional inverse problems (Marcello Carioni, Enschede)
13:20	*CLOSING REMARKS & LUNCH*	

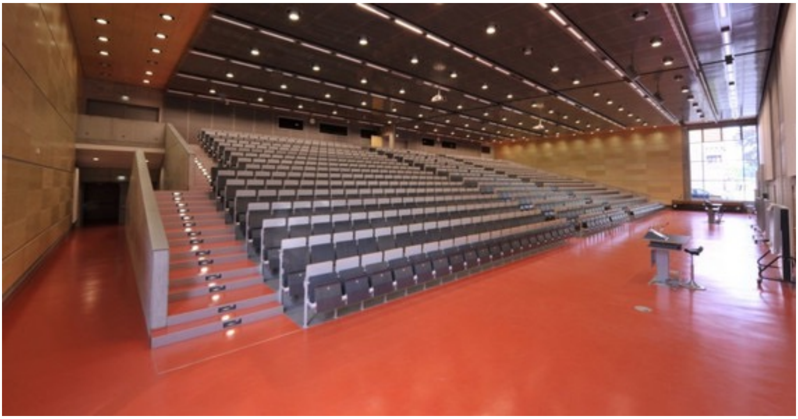
VENUE

The Symposium on Inverse Problems takes place in building 6 at the Campus Griebnitzsee of the University of Potsdam. The Campus Griebnitzsee is well connected to Berlin and Potsdam by train and regional train, as well as by bus. To find the most suitable connection for you, we recommend to use the VBB webpage. Please find the QR code to the VBB webpage below.





The Plenary Talks will take place in the combined lecture hall H03 & H04, whereas parallel sessions will take place in the separated lecture halls H03 and H04. The combined Ice Breaker and the Poster Session will take place in the seminar rooms S12-S16.



Lecture halls H03 and H04, combined (photo by Karla Fritze)

PLENARY SPEAKER

Monday
9:30 am
H03+H04

Tim Salditt | University of Göttingen, DE

Current Challenges in Phase Retrieval and Tomographic Reconstruction: Inverse Problems at Work - An Experimentalist's View

X-rays can provide information about the structure of matter, on multiple length scales from bulk materials to nanoscale devices, from organs to organelle, from the organism to macromolecule. Due to the widespread lack of suitable lenses, the majority of investigations are rather indirect – apart from classical shadow radiography perhaps. While diffraction problems have been solved since long, the modern era has brought about lensless coherent imaging with X-rays, down to the nanoscale. How much more room for improvement is offered by full exploitation of indirect measurements, sophisticated analysis and high performance algorithms, and how far can this go? In this talk we discuss image formation and reconstruction in the optical far- and near-field, the limits imposed by partial coherence, optical constants, and object constraints, the role of imperfect lenses and photon correlations. We show how solutions and algorithms of mathematics of inverse problems help us to meet the challenges of phase retrieval, tomographic reconstruction, and more generally image processing of bulky data. All to the benefit of ambitious imaging projects such as mapping the human brain of fighting infectious diseases.

[1] T. Salditt, A. Egner and R. D. Luke (Eds.) (2020) . Nanoscale Photonic Imaging. Springer Nature, Berlin

[2] S. Huhn, L.M. Lohse, J. Lucht, T. Salditt (2022). Fast algorithms for nonlinear and constrained phase retrieval in near-field X-ray holography based on Tikhonov regularization. arXiv:2205.01099

[3] M. Eckermann, B. Schmitzer, F. van der Meer, J. Franz, O. Hansen, C. Stadelmann and T. Salditt (2021). Three-dimensional virtual histology of the human hippocampus based on phase-contrast computed tomography. Proc. Natl. Acad. Sci., 118, 48, doi:10.1073/pnas.2113835118

Caltech, US | **Elizabeth Qian**

Monday
2 pm
H03+H04

Balanced truncation for Bayesian inference

Qian, E., Tabeart, J., Beattie, C., Gugercin, S., Jiang, J., Kramer, P., and Narayan, A.

Balanced truncation is a system-theoretic method for model reduction which obtains an efficient reduced model by projecting system operators onto state directions which simultaneously maximize observability and minimize reachability. In linear-Gaussian Bayesian inference, an optimal posterior covariance approximation can be made by updating the prior covariance in state directions that are simultaneously maximally informed by the data and minimally precise under the prior. In this talk, we consider the Bayesian inverse problem of inferring the initial condition of a linear dynamical system from noisy output measurements taken after the initial time. We establish natural connections between the Bayesian inferential prior covariance and Fisher information matrix and the system-theoretic reachability and observability Gramians. We use these connections to propose a balancing approach to model reduction for the inference setting. The resulting reduced model then inherits stability properties and error bounds from system theory, and yields an optimal posterior covariance approximation. We hope that these results in the linear setting, obtained via cross-pollination between ideas from system theory and Bayesian inverse problems, will inspire further work bridging these two fields.

[1] Qian, E.; Tabeart, J.; Beattie, C.; Gugercin, S.; Jiang, J.; Kramer, P.; Narayan, A. (2022). Model reduction of linear dynamical systems via balancing for Bayesian inference. Journal of Scientific Computing 91(29).

Tuesday
9 am
H03+H04

Marc Bocquet | CEREA, École des Ponts ParisTech and EDF R & D, FR

Bayesian online algorithms for learning data-driven models of chaotic dynamics

Bocquet, M., Farchi, A., Malartic, Q., Bonavita, M., Laloyaux, P., and Chrust, M.

The exploitation of machine and more specifically deep learning techniques significantly boosts the capabilities of data assimilation and inverse problem techniques used in the geosciences. But it also spurs new, more ambitious goals for data assimilation in high dimensions. Among them, one of the key, currently very popular, area of research consists in learning data-driven models of dynamical systems. With the natural constraints of geoscience, i.e. sparse and noisy observations, this typically requires the joint use of data assimilation methods and neural network representations and tools [1, 2]. However, the vast majority of algorithms are offline; they rely on a set of observations over the physical system, which must be available before the start of the training. We propose new algorithms that update the knowledge of the surrogate (i.e. data-driven) model when new observations are acquired [3, 4]. We carry out this objective with both variational (weak-constraint 4D-Var like) and ensemble filtering (EnKF and IEnKS like) techniques. We successfully test these algorithms on low-order Lorenz models, on quasi-geostrophic models, and on the ERA5 dataset. Remarkably, in several cases, the online algorithms significantly outperform the offline ones. Finally, we discuss the applicability of the variational online method to the improvement of the operational forecast model developed at the ECMWF.

[1] https://www.sciencedirect.com/science/article/abs/pii/S1877750320304725

[2] http://www.aimsciences.org/article/id/eb1e67dd-ccb9-4ab2-8526-15c23feae415

[3] https://www.aimsciences.org/article/doi/10.3934/fods.2020015

[4] https://www.sciencedirect.com/science/article/pii/S1877750321001435

Université Paris, FR | **Gilles Blanchard**

Tuesday
10:20 am
H03+H04

Simultaneous adaptation for several criteria in inverse learning problems using an extendedLepskiĭ principle

In the setting of supervised inverse learning using reproducing kernel methods, we propose a data-dependent regularization parameter selection rule that is adaptive to the unknown regularity of the target function and is optimal both for the least-square (prediction) error and for the reproducing kernel Hilbert space (reconstruction) norm error. It is based on a modified Lepskii balancing principle using a varying family of norms. We also propose an estimation of the noise variance.

ENSAE, IP Paris, FR | **Cristina Butucea**

Tuesday
2 pm
H03+H04

Off-the-grid estimation of sparse mixtures

We consider a general non-linear model where the signal is a finite mixture of an unknown, possibly increasing, number of features issued from a continuous dictionary parameterized by a real non-linear parameter. The signal is observed with Gaussian (possibly correlated) noise in either a continuous or a discrete setup. We propose an off-the-grid optimization method to estimate both the non-linear parameters of the features and the linear parameters of the mixture. We use recent results on the geometry of off-the-grid methods, to give minimal separation on the non-linear parameters such that interpolating certificate functions can be constructed. Using also tail bounds for suprema of Gaussian processes we bound the prediction risk with high probability. Our rates are up to log-factors similar to the rates attained by the Lasso predictor in the linear regression model. We also establish convergence rates that quantify with high probability the quality of estimation for both the linear and the non-linear parameters.
This is joint work with J.F. Delmas, A. Dutfoy and C. Hardy.

Wednesday
9 am
H03+H04

Georg Stadler | NY University, US,

Optimal design of experiments for Bayesian inverse problems governed by PDEs

I will present an overview of optimal experimental design formulations and methods for linear and nonlinear Bayesian inverse problems. A particular focus will be on problems with infinite or high-dimensional parameters, and on how to make computations for these models feasible. I will also discuss challenges arising in problems governed by nonlinear model equations or by models containing inherent uncertainties. Numerical examples from contaminate transport and ground water flow will be used to illustrate the approach and study algorithm performance.

This talk is based on work done in collaboration with Alen Alexanderian, Omar Ghattas, Karina Koval and Noemi Petra.

University of Twente, NL | **Marcello Carioni**

Wednesday
12:50 pm
Hall H04

Sparse optimization methods for infinite-dimensional inverse problems

Carioni, M., Bredies, K., Fanzon, S., Walter, D., Romero, F., Holler, M., Korolev, Y., and Schönlieb, C.

In this talk, I will review several recent results about the sparse optimization of infinite-dimensional inverse problems. First, I will focus on the so-called representer theorems that allow to prove, in the case of finite-dimensional data, the existence of a solution given by the linear combination of suitably chosen atoms. In particular, I will try to convey the importance of such statements in understanding the sparsity in infinite-dimensional settings, describing several possible applications for various relevant problems. In the second part of the talk, I will focus on a sparse optimization algorithm, named generalized conditional gradient method, that is built on the characterization of sparse objects for infinite-dimensional inverse problems. This algorithm is a variant of the classical Frank-Wolfe algorithm, and it does not require an a priori discretization of the domain. I will show convergence results under general assumptions on the inverse problem and finally, I will present some numerical examples in the context of dynamic inverse problems regularized with optimal transport energies.

[1] Bredies, K., & Carioni, M. (2020). Sparsity of solutions for variational inverse problems with finite-dimensional data. Calculus of Variations and Partial Differential Equations, 59(1), 1-26.

[2] Bredies, K., Carioni, M., Fanzon, S. & Romero, F. (2022). A Generalized Conditional Gradient Method for Dynamic Inverse Problems with Optimal Transport Regularization. Found Comput Math (2022). https://doi.org/10.1007/s10208-022-09561-z

[3] Bredies, K., Carioni, M., Fanzon, S. & Walter, D. (2021). Linear convergence of accelerated generalized conditional gradient methods. Arxiv preprint (arXiv:2110.06756)

Wednesday
10:50 am
Hall H04

Nada Cvetkovic | Eindhoven University of Technology, NL

Greedy sensor placement for Bayesian inverse problems via model order reduction

Cvetkovic, N., Aretz, N., Silva, F., and Veroy, K.

Models of physical processes often depend on parameters, such as material properties or source terms, that are only known with some uncertainty. Measurement data can be used to estimate these parameters and thereby improve the model's credibility. When measurements become expensive, it is important to choose the most informative data. This task becomes even more challenging when the model configurations vary and the data noise is correlated. In this work, we consider optimal sensor placement for hyper-parameterized Bayesian inverse problems, where the hyper-parameter characterizes nonlinear flexibilities in the forward model, and is considered for a range of possible values. This model variability needs to be taken into account for the experimental design to guarantee that the Bayesian inverse solution is uniformly informative. In this work we link the numerical stability of the maximum a posterior point and E-optimal experimental design to an observability coefficient that directly describes the influence of the chosen sensors. We propose an algorithm that iteratively chooses the sensor locations to improve this coefficient and thereby decrease the eigenvalues of the posterior covariance matrix. This algorithm exploits the structure of the solution manifold in the hyper-parameter domain via a reduced basis surrogate solution for computational efficiency. The algorithms are suitable for correlated noise models as well as large-scale forward models, achieving computational efficiency through model order reduction.

Monday
10:50 am
Hall H03

Sarah Eberle | Goethe University Frankfurt, DE

Reconstruction of Inclusions in Elastic Bodies Based on Experimental Data

Eberle, S., Harrach, B., and Moll, J.

We take a look at the shape reconstruction of inclusions in elastic bodies and solve the corresponding inverse problem. In doing so, we deal with the rigorously proven theory of the monotonicity methods developed for

linear elasticity with the explicit application of the methods, i.e., the implementation and simulation of the reconstruction of inclusions in elastic bodies for both artificial and experimental data. More specifically, we give an insight into these methods and introduce a lab experiment. Finally, we present our reconstructions based on experimental data and compare them with the simulations obtained from artificial data, where we want to highlight that all inclusions can be detected from the noisy experimental data, thus, we obtain accurate results.

[1] Eberle, S.; Harrach, B. (2021) Shape Reconstruction in Linear Elasticity: Standard and Linearized Monotonicity Method, Inverse Problems, 37 (4), 045006

[2] Eberle, S.; Moll, J. (2021) Experimental Detection and Shape Reconstruction of Inclusions in Elastic Bodies via a Monotonicity Method, Int. J. Solids Struct., 233, 111169

University of Basel, CH | **Yannik Gleichmann**

Wednesday
110:20 am
Hall H03

An Improved Adaptive Spectral Inversion for Inverse Problems

Gleichmann, Y., Baffet, D. H., and Grote, M. J.

A nonlinear optimization method is proposed for inverse scattering problems, when the unknown medium is characterized by one or several spatially varying parameters. The inverse medium problem is formulated as a PDE-constrained optimization problem and solved by an inexact truncated Newton-type method. Instead of a grid-based discrete representation, each parameter is projected to a separate fnite-dimensional subspace, which is iteratively adapted during the optimization. Each subspace is spanned by the first few *stable* eigenfunctions of a linearized regularization penalty functional chosen a priori and additionally its sensitive eigenfunctions, those eigenfunctions that ensure a sufficient decrease of the misfit functional in each step. The small finite number of eigenfunctions effectively introduces regularization into the inversion and thus avoids the need for standard Tikhonov-type regularization and, in practice, appears more robust to missing data or added noise.

Tuesday
11:50 am
Hall H04

Martin Hanke-Bourgeois | Johannes Gutenberg University Mainz, DE

Numerical algorithms for a stochastic realization problem

Hanke-Bourgeois, M., Bockius, N., Shea, J., Jung, G., and Schmid, F.

The generalized Langevin equation is a linear stochastic integro-differential equation and serves as a coarse-grained model from statistical physics for the effective motion of a system of particles, where dissipative forces are represented by a memory kernel. The solution of this equation, e.g., the velocity of a colloid within some solvent is a Gaussian process in time. For effective numerical simulations, physical chemists are interested in an alternative extended Markov model with a number of auxiliary variables, such that the velocity component of this solution approximates well the measured data, i.e., the autocorrelation function of the velocity at an equidistant grid in time. The standard workflow for the solution of this problem consists in (i) solving the inverse problem of reconstructing the memory kernel, and (ii) employing a Padé type approach for determining the matrix entries of the Markov model. We present a new approach which is heading directly for a data-driven extended Markov model by formulating the problem as a stochastic realization problem. Our approach has similarities to the usual model reduction ansatz in the pertinent literature. The main differences consist in the use of time domain data and the need of deriving a passive model. We present numerical examples for the motion of a single colloid in a Lennard-Jones fluid. Data are provided from a molecular dynamics simulation of the all atom system. Then the solvent particles are ignored for the coarse grained model. We show that relatively few (i.e., less than twenty) auxiliary variables are sufficient to determine an extended Markov model which fully captures the dynamics of the colloid. The a posteriori computed memory kernel is in good agreement with those obtained from conventional inverse methods - in fact, our reconstructions seem to exhibit fewer numerical artefacts due to inherent noise in the empirical autocorrelation data than the traditional ones.

[1] Bockius, N.; Shea, J.; Jung, G.; Schmid, F.;Hanke, M. (2021). Model reduction techniques for the computation of extended Markov parameterizations for generalized Langevin equations. J. Phys.: Condens. Matter 33, 214003.

University of Passau, DE | Mareike Hasenpflug

Monday
3:20 pm
Hall H03

Geodesic slice sampling on the sphere

Hasenpflug, M., Habeck, H., Kodgirwar, S., and Rudolf, D.

We introduce a geodesic slice sampler on the Euclidean sphere (in arbitrary but fixed dimension) that can be used for approximate sampling from distributions that have a density with respect to the corresponding surface measure. Such distributions occur e.g. in the modelling of directional data or shapes. Under some mild conditions we show that the corresponding transition kernel is well-defined, in particular, that it is reversible with respect to the distribution of interest. Moreover, if the density is bounded away from zero and infinity, then we obtain a uniform ergodicity convergence result. Finally, we illustrate the performance of the geodesic slice sampler on the sphere with numerical experiments.

[1] Bockius, N.; Shea, J.; Jung, G.; Schmid, F.;Hanke, M. (2021). Model reduction techniques for the computation of extended Markov parameterizations for generalized Langevin equations. J. Phys.: Condens. Matter 33, 214003.

University of Passau, DE | Julian Hofstadler

Tuesday
3:20 pm
Hall H03

Adaptive MCMC for doubly intractable distributions

Bayesian inference in the context of biophysical problems may lead to posterior densities with two unknown quantities, the normalizing constant and an intractable multiplicative factor in the likelihood function. Not being able to evaluate the likelihood function leads to computational issues in classical (adaptive) MCMC algorithms and in the past years various methods have been suggested to overcome this problem. We discuss an adaptive MCMC scheme that relies on approximating the likelihood function and, moreover, we present a strong law of large numbers for mounded measurable functions.

Tuesday
11:20 am
Hall H04

Simon Hubmer | Johann Radon Institute Linz, AT

Subaperture-based Digital Aberratio Correction for OCT

Hubmer, S., Sherina, E., and Ramlau, R.

In this talk, we consider subaperture-based approaches for the digital aberration correction (DAC) of optical coherence tomography (OCT) images. In particular, we introduce a mathematical framework for describing this class of approaches, which results in a new understanding of the previously introduced subaperture-correlation method. Furthermore, based on the insight gained by this mathematical description, we present a novel DAC approach requiring only minimal statistical assumptions on the spectral phase of the scanned object. Finally, we demonstrate the applicability of our novel DAC method via numerical examples based on both simulated and experimental OCT data.

Wednesday
12:50 pm
Hall H03

Tim Jahn | University of Bonn, DE

Discretisation-adaptive regularisation of statistical inverse

We consider linear inverse problems under white (non-Gaussian) noise. We introduce a discretisation scheme to apply the discrepancy principle and the heuristic discrepancy principle, which require bounded data norm. Choosing the discretisation dimension in an adaptive fashion yields convergence, without further restrictions for the operator, the distribution of the white noise or the unknown ground solution.

[1] Jahn, T. (2022). Optimal convergence of the discrepancy principle for polynomially and exponentially ill-posed operators under white noise. Numer.Funct. Anal. Optim. 43(2), p.145-167, doi:10.1080/01630563.2021.2013881
[2] Jahn, T. (2022). A probabilistic oracle inequality and quantification of uncertainty of a modified discrepancy principle for statistical inverse problems. Electron. Trans. Numer. Anal. 57, p.35-56, doi:10.1553/etna_vol57s35
[3] Jahn, T. (2022). Discretisation-adaptive regularisation of statistical inverse problems. arXiv:2204.14037

University of Klagenfurt, AT | **Barbara Kaltenbacher**

Wednesday
10:50 am
Hall H03

Some inverse problems for wave equations with fractional derivative attenuation

Kaltenbacher, B., and Rundell, B.

A characteristic property of ultrasound propagating in human tissue is frequency power law attenuation leading to fractional derivative damping models in time domain. In this talk we will first dwell on fractional damping models and their analysis. Then we will discuss related inverse problems such as the reconstruction of the initial pressure as relevant as a subproblem of photoacoustic tomography. In particular we highlight dependence of ill-posedness on the strength of damping, that is, on the order of the fractional derivative. The damped wave equation with the attenuation proportional to velocity is ubiquitous in science and engineering and a common situation is when the attenuation depends on frequency. The usual way to incorporate this effect is to introduce fractional order derivatives either as a replacement for u_t or as modifier through a spatial component with space fractional derivatives. Models for these are very well developed and the effort in this paper is towards the analysis of the inverse problem of recovering critical coefficients or initial states although we also develop constructive methods for these and analyse their degree of ill-conditioning.

Barbara Kaltenbacher and William Rundell. Some inverse problems for wave equations with fractional derivative attenuation. Inverse Problems, 37(4):045002, mar 2021.

University of Siegen, DE | **Chantal Klinkhammer**

Wednesday
12:20 pm
Hall H03

Tikhonov Regularization - Low order convergence Rates for a discrepancy principle under low order source conditions in the oversmoothing case

Klinkhammer, C., and Plato, R.

We study the application of Tikhonov Regularization on ill-posed nonlinear operator equations. The object of this work is to prove low order convergence rates for the discrepancy principle under a specific low order source condition of logarithmic type. We work within the framework of Hilbert scales and extend existing studies on this subject to the oversmoothing case, which means that the exact solution fails to have a finite penalty functional since it does not belong to its domain of definition.

Monday
3:20 pm
Hall H04

Tomáš Kocák | University of Potsdam, DE

Multi-armed bandit problem with side observations

Many real-world problems, such as movie recommendations, clinical trials, and ad placement, are sequential in nature. The learner is presented with a set of actions, picks one of the actions, and receives a reward for the action. The objective is to accumulate as much reward over time as possible. Traditionally, the actions are independent. This assumption might be too restrictive in some applications. Therefore, in this talk, we focus on the problem with an underlying graph structure where actions are vertices and picking an action reveals rewards of all its neighbors.

T. Kocák, G. Neu, M. Valko, and R. Munos. Efficient learning by implicit exploration in bandit problems with side observations. In Advances in Neural Information Processing Systems

Wednesday
11:20 am
Hall H04

Karina Koval | University of Heidelberg, DE

Optimal design of experimental conditions for a Bayesian inverse problem in photoacoustic imaging

Koval, K., Herzog, R., and Scheichl, R.

Photoacoustic imaging (PAI) is a rapidly developing non-invasive imaging modality that enables visualization of optical tissue properties with rich contrast and high spatial resolution. In PAI an object is illuminated with a short light pulse, causing a localized rise in pressure that propagates through the tissue and is measured by transducers on the boundary. Typically, these noisy observations are used to infer relevant optical and acoustic properties of tissues through the solution of two coupled inverse problems. One major challenge inhibiting the estimation of these parameters is the various uncertainties present in the partial differential equations used to model the propagation of light and pressure through the medium. Additionally, transducer geometries and physical constraints hinder data acquisition and lead to regions with high uncertainty in the parameter reconstructions. Employing a Bayesian approach to a PAI inverse problem, we focus on design of experimental conditions that lead to optimal reconstructions of tissue properties while incorporating inherent model uncertainties.

University of Würzburg, DE | **Remo Kretschmann**

Monday
4:20 pm
Hall H03

Bayesian hypothesis testing in statistical inverse problems

Kretschmann, R., and Werner, F.

In many inverse problems, one is not primarily interested in the whole solution $u^\dagger \in X$, but in specific features of it that can be described by a family of linear functionals of $u^\dagger$. We perform statistical inference for such features by means of hypothesis testing. This problem has recently been treated by multiscale methods based upon unbiased estimates of those func- tionals [1]. Constructing hypothesis tests using unbiased estimators, however, has two severe drawbacks: Firstly, unbiased estimators only exist for sufficiently smooth linear functionals, and secondly, they suffer from a huge variance due to the ill-posedness of the problem, so that the corresponding tests have bad detection properties. We overcome both of these issues by considering the problem from a Bayesian point of view, assigning a prior distribution to $u^\dagger$, and using the resulting posterior distribution to define regularized hypothesis tests. We study this approach both analytically and numerically for linear inverse problems and compare it with unregularized hypothesis testing.

[1] K. Proksch; F. Werner; A. Munk (2018). Multiscale scanning in inverse problems. Ann. Statist., 46(6B), p.3569–3602, doi:10.1214/17-AOS1669

University of Potsdam, DE | **Han Cheng Lie**

Tuesday
3:50 pm
Hall H03

Overconfidence and randomisation in numerical Bayesian inverse problems

Lie, H. C., Stahn, M., Sullivan, T. J., and Teckentrup, A.

Many physics-based models of natural phenomena are expressed in terms of differential equations. These models are often subject to uncertainty because they depend on parameters that are not known precisely, such as initial conditions, boundary conditions, or coefficients in the differential equation. Another source of uncertainty is unresolved scales, e.g. in weather prediction. To make predictions about the natural phenomenon of interest, one must first perform inference for the unknown parameters using noisy, incomplete observations of the solution to the differential equation, and then calibrate the model using these parameter values. Bayesian approaches to solving such inference problems involve encoding available knowledge about the unknown parameter into a prior probability measure, and then assimilating the information in data into the posterior probability measure by using Bayes' formula. For differential equation-based models, drawing a single sample from the posterior requires computing the solution of the differential equation. In practice, the differential equation can be solved only numerically. If the numerical solution contains an approximation error, then the resulting approximate posterior can be overconfident, in the sense that the bias between the posterior mean and the true parameter is large relative to the variance. We shall present an analytical example that illustrates how overconfidence can arise due to the approximation error of a numerical solver, and how randomisation of the numerical solver can help to mitigate the problem of overconfidence. If time permits, we shall state theoretical results concerning error bounds for randomised approximate numerical solvers for initial value problems defined on Gelfand triples, and connect these to error bounds for posterior measures corresponding to randomised approximate forward models.

[1] Lie, H. C.; Stahn, M.; Sullivan, T. J. (2022). Randomised one-step time integration methods for deterministic operator differential equations. Calcolo 59(13), doi:10.1007/s10092-022-00457-6

[2] Lie, H.C.; Sullivan, T.J.; Teckentrup, A.L. (2018). Random forward models and log-likelihoods in Bayesian inverse problems. SIAM/ASA J. Uncertain. Quantif. 6(4), p.1600-1629, doi:10.1137/18M1166523

Monday
11:20 am
Hall H03

Bochra Mejri | Johann Radon Institute Linz, AT

Quantitative elastic diffraction tomography

In this work, we consider an elastic diffraction tomography problem for propagated and evanescent waves. More precisely, we are interested to reconstruct, quantitatively, the elastic properties (i.e. mass density and elastic Lamé parameters) for a weakly scattering object embedded in an

elastic full-space. Firstly, the elastic inverse scattering problem under consideration is linearized using the first-order Born approximation. Then, the Fourier diffraction theorem is proved in the distributional sense for transmission or reflection acquisitions. Wave mode separation is performed using the properties of the P- and S- waves and specific filters defined by the propagation vectors. A new multi-parameter inversion process is developed in the Fourier domain. Back-propagation formulae is established for different modes (PP,PS,SP,SS) with measurements in rotated observations space. Different coverages of k-space are obtained in terms of angular diversity by varying the illumination direction for a fixed frequency.
This is a joint work with Otmar Scherzer.

University of Göttingen, DE | Philipp Mickan

Tuesday
3:50 pm
Hall H04

Variational Source Condition for an Inverse Source Problem

Mickan, P., and Hohage, T.

In this presentation we will discuss the inverse source problem to determine the strength of a random acoustic sound source by correlation data generated by the observation of the pressure signal of the emitted time harmonic acoustic waves. This model can be applied to aeroacoustics where regularisation methods for the inverse source problem constitute the best approach to determine a sound source. As uniqueness has been recently proven for this problem one naturally investigates the stability properties. This presentation hence contains as one of the main result a rigorous proof of a logarithmic convergence rate for the Tikhonov regularisation applied to the inverse source problem. This result is obtained by verifying a variational source condition by methods developed by Hohage and Weidling. Therefore, we establish stability estimates using geometrical optics solutions.

MPI for Solar System Research, DE | Björn Müller

Wednesday
10:20 am
Hall H04

Solving a quantitative passive imaging problem in helioseismology by iterative holography: Inversions for solar differential rotation

Müller, B., Hohage, T., Fournier, D., and Gizon, L.

We study the passive imaging problem of estimating parameters in the solar interior from cor- relation measurements of line-of-sight velocities at the solar surface. In the frequency domain the cross-correlation data takes the form C(r1,r2,ω) = ψ(r1,ω)∗ψ(r2,ω) with freqeuency ω and two points r1,r2 on the solar surface. The solar surface is observed on CCD grid with 4096x4096 points which leads to approximately 1014 independent correlation pairs for each frequency. This shows that the extremly noisy five-dimensional data set is unfeasible to store and invert directly leading to a need in apriori averaging in space and frequency. Helioseismic holography performs these averages due to physical motivated backpropagation of the surface fluctuations into the solar interior [1]. In this talk we describe the holographic backpropagation as Fréchet derivative of a particular operator mapping to the covariance data at the solar surface [2]. We develop a theoretical framework for holography-based inversions which allows us to extend holography to a full quantitative iterative regularization method. By changing the order of backpropagation and correlation we can use the whole cross-correlation data implicitly by avoiding the computation explicitly. Furthermore once the forward prob- lem is solved the adjoint and the derivative can be computed efficiently by manipulating the right hand side. Finally this approach allows us to tackle nonlinear inverse problems in helioseismology. Nonlinear inversions are usually not studied by traditional approaches like time-distance helioseismology due to the high computational costs occuring from the strong gradients in the solar atmosphere [3]. In particular we present inversion results for axisym-metric flows which play a significant role in solar dynamo theory. Traditional inversions based on frequency shifts lack in reconstructing the north-south antisymmetric differential rotation profile. This problem can be solved with iterative holography.

[1] Lindsey, C; Braun, D. (1997). Helioseismic Holography. Astrophysical Journal 485(2), p.895-903, doi:10.1086/304445

[2] Hohage, T.; Raumer, H.; Spehr C. (2020). Uniqueness of an inverse source problem in experimental aeroacoustics. Inverse Problems 36(7), doi:10.1088/1361-6420/ab8484

[3] Gizon, L. et. al. (2017). Computational helioseismology in the frequency domain: acoustic waves in axisymmetric solar models with flows. Astronomy and Astrophysics 600, A35, doi:10.1051/0004-6361/201629470

University of Graz, AT | Tram Nguyen

Tuesday
5:20 pm
H03 & H04

A model reference adaptive system approach for nonlinear online parameter identification

Nguyen, T., and Kaltenbacher, B.

Dynamical systems, for instance in model predictive control, often contain unknown parameters, which must be determined during system operation. The challenge of online methods is that one must continuously estimate parameters as experimental data becomes available. The existing techniques for time-dependent partial differential equations exclude the case where the system depends nonlinearly on the parameters. Based on a model reference adaptive system approach, we present an online parameter identification method, which works for nonlinear infinite-dimensional evolutionary systems.

Norwegian University of Life Sciences, NO | Bjørn Fredrik Nielsen

Tuesday
3:20 pm
Hall H04

Weighted regularization for identifying sources from Cauchy boundary data

Nielsden, B. F., and Elvetun, O. L.

We consider the problem of identifying a source in an elliptic PDE from Cauchy boundary data. If standard regularizations methods are employed, then the computed source will always be positioned at the boundary, even when the true source is interior. This is due to the nontrivial null space of the associated forward operator, and we propose a weighting procedure/regularization operator to rectify this. In the first part of the talk, after defining the new regularization operator, we will consider weighted Tikhonov regularization. Our analysis and experiments show that the new scheme correctly recovers the position of the source, regardless of its true location. Nevertheless, the inverse solution is very smooth, and the source is "smeared out" compared with the true one. It turns out that weighted sparsity regularization, combined with box constraints, can enable rather accurate recovery of sources with constant magnitude/strength, which is the topic of the second part of our talk. In addition, for sources with varying strength, the support of the inverse solution will be a subset of the support of the true source. We present both some theoretical results and numerical experiments. Our work only addresses discretized problems. This investigation is motivated by ECG and EEG applications. However, we develop the theory in terms of Euclidean spaces and the methodology can therefore be applied to many problems. For example, the results are equally applicable to models involving the screened Poisson equation as to models using the Helmholtz equation, with both large and small wave numbers.

Tuesday
11:50 am
Hall H03

Jan-Frederik Pietschmann | TU Chemnitz, DE

Data driven gradient flows

Pietschmann, J.-F.., and Schlottbom, M.

We present a framework enabling variational data assimilation for gradient flows in general metric spaces, based on the minimizing movement (or Jordan-Kinderlehrer-Otto) approximation scheme. We focus on the space of probability measures endowed with the Wasserstein distance as thiscovers many non-linear partial differential equations (PDEs), such as the porous medium equation or general drift-diffusion-aggregation equations, which can be treated by our methods independent of their respective properties (such as finite speed of propagation or blow-up). We present a numerical implementation of our approach using an primal-dual algorithm. The strength of our approach lies in the fact that by simply changing the driving functional, a wide range of PDEs can be treated without the need to adopt the numerical scheme. We conclude by presenting detailed numerical examples.

Tuesday
4:20 pm
Hall H03

Mihaela Pricop-Jeckstadt | University POLITEHNICA of Bucharest, RO

Optimal rates of convergence for functional data analysis with indirect observations

We focus in this paper on the optimal parameter estimation from noisy independent realizations of a stochastic process that is indirectly observed [1,2,3]. First, we study minimax rates of convergence for a class of linear inverse problems with correlated noise, general source conditions and various degrees of ill-posedness for entirely observed pathes. In the

In the framework of the projected data, two settings are presented separately: the case of the common design (when the set of test functions are all identical) and the case of the independent design. The latter reduces to the former under the specific conditions of the common design and has an interpretation in the view of the sampling properties via s-numbers [4,5]. The phase transition can be observed also here as it is usual for the functional data analysis. We compute the thresholds that separate the sparse and the dense data set settings for different smoothness conditions, compare the optimal rates of convergence in different scenarios with the rates corresponding to the statistical inverse problems and observe that the price to pay for the data correlation proves to be high [6]. Finally, the rates of convergence of the Tikhonov regularization applied to Abel's integral equation are numerically illustrated in different settings.

[1] Minimax Rates for Statistical Inverse Problems Under General Source Conditions, Ding, L. and Mathé, P., Computational Methods in Applied Mathematics 18 (2017)

[2] Optimal discretization of inverse problems in Hilbert scales. Regularization and self-regularization of projection methods, Mathé, P. and Pereverzev, S., SIAM J. Numer. Anal. 38 (2001)

[3] Convergence rates of general regularization methods for statistical inverse problems and applications, Bissantz, N. and Hohage, T. and Munk, A. and Ruymgaart, F., SIAM Journal on Numerical Analysis 45 (2007)

[4] Optimal estimation of the mean function based on discretely sampled functional data: Phase transition, T. T. Cai and M. Yuan, Annals of Statistics 39 (2011)

[5] From sparse to dense functional data and beyond, Zhang, X. and Wang, J.L., Annals of Statistics 44 (2016) [6] Optimal indirect estimation for linear inverse problems with discretely sampled functional data, MPJ, Inverse Problems 37 (2021)

TU Berlin, DE | Michael Quellmalz

Wednesday
11:20 am
Hall H03

Optical diffraction tomography with an object rotated into arbitrary orientations

Quellmalz, M., Beinert, R., Elbau, P., Kirisits, C., Scherzer, O., and Steidl, G.

We study the mathematical imaging problem of optical diffraction tomography (ODT) for the scenario of a rigid particle rotating in a trap created by acoustic or optical forces. Under the influence of the inhomogeneous forces, the particle carries out a time-dependent smooth, but irregular motion. The rotation axis is not fixed, but continuously undergoes some variations, and the rotation angles are not equally spaced, which is in contrast to standard tomographic reconstruction assumptions. Once the time-dependent motion parameters are known, the particle's scattering potential can be reconstructed based on the Fourier diffraction theorem, considering it is compatible with making the first order Born or Rytov approximation.

Tuesday
11:20 am
Hall H03

William Rundell | Texas A & M University, US

On Recovering the Fractional Damping Operator in a Wave Equation from Time Trace Data

Rundell, W., and Kaltenbacher, W.

This talk deals with the inverse problem of recovering a multi-term fractional damping operator in a wave equation. We develop several approaches on uniqueness and reconstruction, some of them relying on Tauberian theorems that provide relations between theasymptotic behaviour of solutions in time and Laplace transform domains. The possibility of additionally recovering space-dependent coefficients or initial data is discussed. The resulting methods for reconstructing coefficients and fractional orders in these terms are tested numerically and we give an indication of the underlying analysis of both the forwards and the inverse problem.

B. Kaltenbacher and W. Rundell, Determining damping terms in fractional wave equations, Inverse Problems 38 075004, 2022.

Tuesday
11:20 am
Hall H03

Naomi Schneider | University of Siegen, DE

Learning a regularized solution from infinitely many trial functions

In the geosciences, ill-posed inverse problems are often the underlying mathematical problem to be solved: for instance, if we aim to approximate the gravitational potential via the downward continuation of satellite data or seek insight into the interior of the Earth via the travel time tomography using earthquake data.

Both challenges are important in order to monitor certain influences on the system Earth, in particular the mass transport of the Earth or its geomagnetic field.

MPI for Multidisciplinary Sciences, DE | Steffen Schultze

Monday
3:50 pm
Hall H03

Bayesian Structure Determination from Single Molecule X-Ray Diffraction

Schultze, S., and Grubmüller, H.

Single molecule X-Ray diffraction experiments are a promising new method for the structure determination of biomolecules. The reconstruction of the structure from these experiments is quite challenging: The scattering images are sparse, each containing only 10-50 photons on average, and the signal to noise ratio is very low. In addition, the orientations of the molecules at the time of scattering are unknown. Available analysis methods require at least 100 photons per image, or a very large number (e.g. 10^9) of images. We present a novel Bayesian approach that requires fewer photons per image and, at the same time, relatively few images. It is flexible in that many different representations of the electron density can be used, both in Fourier space and directly in real space. Using synthetic data, we demonstrate the method is able to recover the structure of the protein crambin at 6-7Å resolution using only 10^6 images, and at 3.8Å resolution using 10^8 images.

Saarland University, DE | Thomas Schuster

Tuesday
4:20 pm
Hall H04

Ill-posedness of time-dependent inverse problems in Lebesgue-Bochner spaces

Schuster, T., Burger, M., and Wald, A.

We call an inverse problem time-dependent, if the given data and / or the searched parameters depend on time. This class of problems comprises applications such as dynamic computer- ized tomography, dynamic MRI, magnetic particle imaging or dynamic load monitoring in elasticity. Usually the time variable is defined as an additional dimension equally with the spatial dimensions though there are good reasons to see it as a variable on its own. E.g., weak solutions of parabolic or hyperbolic equations have different regularities in time and space. But an holistic theoretical and numerical framework for time-dependent inverse problems is still missing. In the talk we discuss the phenomenon of ill-posedness for linear operators $F : \mathbf{X} \to \mathbf{Y}$ in Lebesgue-Bochner spaces $\mathbf{X} = L^p(0,T;\mathcal{X})$, $\mathbf{Y} = L^q(0,T;\mathcal{Y})$ where $\mathcal{X}$, $\mathcal{Y}$ are Banach spaces. We introduce the concepts of temporally and uniformly ill-posedness and demonstrate their differences when F is given by time-dependent observations of a compact operator, a setting which is appropriate for many real world applications. Adopted to these concepts we define temporal and uniform regularization methods. These could be first steps towards an integrative framework for tackling time-dependent inverse problems. This is joint work with Martin Burger (University of Erlangen) and Anne Wald (University of Göttingen).

Wednesday
12:20 pm
Hall H04

Lisa Schwetlick | University of Potsdam, DE

Modelling Eye Movement: What DNNs And Biological Models Can Teach Each Other

Schwetlick, L., Kümmerer, M., Bethge, M., and Engbert, R.

When looking at natural scenes humans move their eyes in a sequence of fixations and saccades. The selection of each subsequent location depends on a variety of factors ranging from image content to eye movement dynamics and sequential dependencies. Recent research has seen a variety of models that aim to predict time-ordered scan paths. Popular modelling frameworks such as statistical, mechanistic as well as deep neural network (DNN) models each have their own advantages and shortcomings. Leveraging the strength of different frameworks may allow us to gain new insights into the processes that underlie fixation selection. DNN models, relying on thousands of parameters, are highly performant and learn to account for much of the variance in the data. Biological models on the other hand are highly interpretable and allow researchers to understand underlying mechanisms. Here we show that we can use DNNs to estimate the predictability of the data and use them to uncover unaccounted mechanisms in the biological model. Furthermore the biological model can help develop an understanding of mechanisms learned by DNNs. DeepGaze3 (DG3) is currently the best-performing DNN model for scan path predictions (Kümmerer & Bethge, 2020); SceneWalk (SW) is the best-performing biologically inspired dynamical model (Schwetlick et al., 2021).

As both models are likelihood-based, we can evaluate the predictability of each fixation and analyze highly divergent cases on a fixation-by-fixation basis. Using this approach we identify specific situations where DG3 consistently outperforms SW, and draw conclusions about potentially missing mechanisms. For example, preliminary results show that SW tends to underestimate the probability of long, explorative saccades. By adding a corresponding mechanism to SW, we were able to improve model performance. Thus, we are able to use insights from the comparison to build more advanced and performant dynamical models. We conclude that finding synergies between different modeling approaches not only usefully combines expertise from different fields but is a valuable tool for improving our understanding of fixation selection during scene viewing.

University of Potsdam, DE | **Karen Seidel**

Monday
3:50 pm
Hall H04

Sequential Learning

In machine learning, algorithms generalize from available training data to unseen situations. The engineering practices used in the respective technologies are far from understood. Research in theoretical machine learning analyses concrete mathematical models for this complex subject. We investigated models for incremental binary classification, an example for supervised sequential learning. Moreover, we introduce a class of sequential learning algorithms suitable for improving Data Sampling. Bandit Algorithms have been developed for resolving the exploration versus exploitation trade-off when navigating with incomplete information in an uncertain environment. We consider discrete and continuous versions in the context of dependencies in the sampling process.

[1] Seidel, K. (2021). Modelling binary classification with computability theory (Doctoral dissertation, Universität Potsdam).

[2] Zadorozhnyi, O., Blanchard, G., & Carpentier, A. (2019). Restless dependent bandits with fading memory. arXiv preprint arXiv:1906.10454.

[3] Bubeck, S., Stoltz, G., Szepesvári, C., & Munos, R. (2008). Online optimization in X-armed bandits. Advances in Neural Information Processing Systems, 21.

Monday
11:50 am
Hall H04

Bernadett Stadler | Johannes Kepler University Linz, AT

An augmented Krylov subspace method for atmospheric tomography

Stadler, R., and Ramlau, R.

Atmospheric tomography, i.e. the reconstruction of the turbulence profile in the atmosphere, is a challenging task for adaptive optics (AO) systems of the next generation of Extremely Large Telescopes (ELTs). Mathematically, the reconstruction of turbulent layers in the atmosphere is ill-posed. Moreover, the reconstruction has to be performed in real-time. For large systems, such as the ELT of the European Southern Observatory (ESO), the atmospheric tomography problem is considerably complex and the computational efficiency becomes an issue. In this talk we consider an iterative solver for atmospheric tomography, called augmented Finite Element Wavelet Hybrid Algorithm (FEWHA). The inverse problem is regularized using the Bayesian framework and the maximum a posteriori estimate. The algorithm applies a discretization with a wavelet and bilinear basis, which yields sparse operators. The sparse system is solved with the well-known preconditioned conjugate gradient (PCG) method. A crucial indicator for the real-time performance of augmented FEWHA is the number of PCG iterations. We apply an augmented Krylov subspace method, which allows to decrease the number of iterations significantly. The quality of our algorithm is validated via numerical simulations for the ELT's instrument MAORY. We demonstrate that a parallel, matrix-free implementation of augmented FEWHA fulfills the quality and real-time requirements of ESO's ELT.

[1] B. Stadler, R. Ramlau (2021). An augmented wavelet reconstructor for atmospheric tomography. Electron. Trans. Numer. Anal., 54.

[2] B. Stadler, R. Biasi, M. Manetti and R. Ramlau (2019). Feasibility of standard and novel solvers in atmospheric tomography for the ELT. In Proceedings AO4ELT6 Conference.

[3] B. Stadler, R. Biasi, M. Manetti, R. Ramlau (2021). Parallel implementation of an iterative solver for atmospheric tomography. In Proceedings 21th International Conference on Computational Science and Its Applications (ICCSA).

[4] B. Stadler and R. Ramlau (2022). Performance of an iterative wavelet reconstructor for the Multi-conjugate Adaptive Optics RelaY of the ELT. Journal of Astronomical Telescopes, Instruments, and Systems (JATIS), 8.

University of Heidelberg, DE | **Simon Weissmann**

Monday
11:20 am
Hall H04

Multilevel Optimization for Inverse Problems

Weissmann, S., Wilson, A., and Zech, J.

In this talk, we introduce a unifying framework of multilevel optimization schemes that can be applied to a wide range of optimization-based solvers arising in inverse problems. The proposed framework provably reduces computational costs associated to the evaluation of a complex forward map stemming from physical models. We demonstrate the versatility of our approach through the application to various methodologies including multilevel (accelerated) stochastic gradient descent, a multilevel ensemble Kalman inversion and a multilevel Langevin sampler.

[1] Weissmann, S.; Wilson A.; Zech J. (2022). Multilevel Optimization for Inverse Problems. Proceedings of Thirty Fifth Conference on Learning Theory, PMLR 178:5489-5524.

University of Hamburg, DE | **Lena Zdun**

Monday
10:50 am
Hall H04

Challenges of dynamic data: joint reconstruction and motion estimation in MPI

Zdun, L., Brandt, C., and Kluth, T.

Magnetic Particle Imaging (MPI) is a pre-clinical tracer-based tomographic imaging method with numerous potential applications. It is non-invasive and doesn’t use ionizing radiation, however it has high spatial and temporal resolution. Potential applications include dynamic imaging tasks as blood flow imaging and instrument tracking during interventions, where not only the reconstructed images but also the motion in-between image frames is of interest. However, the image reconstruction task which is already severely ill-posed in case of static data poses an even more challenging problem in case of dynamic data and motion estimation in 3D is highly underdetermined. We expect results of higher quality for both tasks when solving the image reconstruction task jointly with the motion estimation, as both processes endorse each other [1]. Different motion models are used depending on the specific application. We start from a fairly general variational problem formulation and exploit prior knowledge to adapt the formulation to the setting of MPI reconstruction. The problem is solved by primal-dual splitting algorithms using stochastic algorithmic approaches, multi-scale approaches and warping. We present numerical results on simulated data for different phantoms and motion.

[1] Burger, M.; Dirks, H.; Schönlieb, C.- B. (2018). A Variational Model for Joint Motion Estimation and Image Reconstruction. SIAM Journal on Imaging Sciences 11(1), p. 94–128, doi:10.1137/16M1084183

University of Potsdam, DE | **Diksha Bhandari**

Neural network modelling of brain responses during language comprehension

Bhandari, D., and Reich, S.

Advances in machine learning have highlighted the tools for reconstruction of the dynamics of an observed physical system as a surrogate model. Recent studies have shown that data- driven methods exhibit remarkable success in reproducing complex spatiotemporal processes, and have therefore been used in an increasing number of applications. The most commonly used such architectures include random forests, echo state networks, recurrent and convolutional neural networks.The goal of most of these methods is to minimize the loss function which is a measure of the discrepancy between the observation dataset and the statistical model predictions. As a separate field of research, Data assimilation is used as a technique that aims to find the best possible estimate of a dynamical system based on past observations. One of the most famous and robust methods for data assimilation is the Ensemble Kalman filter (EnKF), introduced by Evensen in 1994. The key idea of this work is to combine machine learning methods with data assimilation to reconstruct a dynamical system. We use a scaled-up version of the Sentence Gestalt (SG) model, a neural network model of sentence comprehension and investigate the appropriateness of Bayesian learning algorithms for training. For this setting, affine-invariant extensions of the Ensemble Kalman Filter (EnKF) and related methods to the cross-entropy loss function are used as alternative correlation based optimizers when training a deep learning model.

[1] Pidstrigach, J., Reich, S. Affine-Invariant Ensemble Transform Methods for Logistic Regression. Found Comput Math (2022). https://doi.org/10.1007/s10208-022- 09550-2

[2] Rabovsky M, Hansen SS, McClelland JL. Modelling the N400 brain potential as change in a probabilistic representation of meaning. Nat Hum Behav. 2018 Sep;2(9):693-705. doi: 10.1038/s41562-018-0406-4. Epub 2018 Aug 27. PMID: 31346278.

[3] Lopopolo, A., & Rabovsky, M. (2021). Predicting the N400 ERP component using the Sentence Gestalt model trained on a large scale corpus. Proceedings of the Annual Meeting of the Cognitive Science Society, 43.

Katherine Briceno Guerrero | University of Potsdam, DE

Efficient parametrization of optimal dosing schemes: Neural Network as a surrogate for the Reinforcement Learning Action-Value Function

Briceno Guerrero, K., Opper, M., Hartung, N., Huisinga, W., and de Wiljes, J.

In many application areas, there is a need to determine a control variable that optimizes a prespecified objective. This problem is particularly challenging when knowledge of the underlying dynamics is subject to various sources of uncertainty and access to observations is severely limited. A scenario such as that for example arises in the context of therapy individualization to improve the efficacy and safety of medical treatment. Mathematical models describing the pharmacokinetics and pharmacodynamics of a drug together with data on associated biomarkers can be leveraged to support decision-making by predicting therapy outcomes. We present a continuous learning strategy that allows us to sequentially update the model parameters and states via a particle-based data assimilation scheme and combine it with reinforcement learning to tailor the dosing policy to the specific patient [1]. We explore different schemes to parametrize the policy as well as the expected long-term reward in order to deal with the high dimensional action and state space [2,3,4]. As these parameterizations may increase the overall uncertainty we explore how they are reflected in the approximated control variable.

[1] Maier C. et. al (2021). Reinforcement learning and Bayesian data assimilation for model-informed precision dosing in oncology. CPT:PSP.

[2] Sutton, R. S., & Barto, A. G. (2018). Reinforcement learning: An introduction. MIT Press

[3] Dong H. et. al (2020) Deep Reinforcement Learning: Fundamentals, Research, and Applications. Springer.

[4] Bishop et. al (2006). Pattern Recognition and Machine Learning. Springer

Angelica Maria Castillo Tibocha| GFZ, DE

Ensemble data assimilation techniques for electron phase space density in the radiation belts

Castillo Tibocha, A., M., de Wiljes, J., Shprits, Y. Y., and Aseev, N. A.

Accurate predictions of the effects of hazardous energetic solar plasma events on the near-Earth space environment are invaluable to prepare for and potentially prevent harmful implications to humans and technology in space and on the ground.

In order to obtain accurate predictions despite uncertainties in the associated model and the observations, novel data assimilation methods have become increasingly popular. The associated inference problem is particularly challenging when wave activity and mixed diffusion are taken into account, such that the underlying system becomes non-linear. In this case, robust techniques for high dimensional settings are asked for. The class of ensemble Kalman filters has been shown to be one of the most promising filtering tools for non-linear and high dimensional systems in the context of terrestrial weather prediction but has been barely used in the context of electron phase space density for the outter radiation belt. In this study, we adapt traditional ensemble based methods to reduce uncertainties in the estimation of electron phase space density. We use a one-dimensional radial diffusion model, a standard Kalman filter (KF) and synthetic data to setup the framework for one-dimensional ensemble data assimilation. Furthermore, with the split-operator technique, we develope a total of three split-operator Ensemble Kalman filter approaches for electron phase space density in the radiation belts. The capabilities and properties of the proposed filter approaches are verified on Van Allen Probe and GOES data. Additionally, we compare the performance, computational feasability and output of these three split-operator Ensemble Kalman filters with the simulations of a full 3D-Ensemble Kalman filter (including mixed terms).

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University of Potsdam, DE | **Giuseppe Carere**

Reduced basis methods for random PDEs and control problems governed by PDEs

Carere, G., Strazzullo, M.,Ballarin, F., Rozza, G., and Stevenson, R.

Reduced basis approximations of Optimal Control Problems (OCPs) governed by steady partial differential equations (PDEs) with random parametric inputs are analyzed and constructed.

Such approximations are based on a Reduced Order Model, which in this work is constructed using the method of weighted Proper Orthogonal Decomposition. This Reduced Order Model then is used to efficiently compute the reduced basis approximation for any outcome of the random parameter. We showed that a step in the construction of these Reduced Order Models, known as the aggregation step, is not fundamental and can in principle be skipped for noncoercive problems, leading to a cheaper online phase. Numerical applications from environmental science are considered, in which the governing PDE is steady and the control is distributed. Various parameter distributions are taken, and several implementations of the weighted Proper Orthogonal Decomposition are compared by choosing different quadrature rules.

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Agniva Datta | University of Potsdam, DE

Inferring Active Particle Dynamics by Data Assimilation

Datta, A., Albrecht, J., Großmann, R., Beta, C., and Opper, M.

How to systematically infer dynamical models of actively driven entities based on their trajectory data, is a long-standing question in the field of active matter. Understanding bacterial motility serves as an essential candidate for solving this riddle. Using Pseudomonas putida, a rod-shaped gram-negative soil bacterium as a model organism, we work at the interface of stochastic modeling, statistical inference and data assimilation to develop a modeling framework for its complex, stochastic motility patterns. We concentrate on the following question: How does bacterial communication via density-dependent chemical signals (quorum sensing) affect their different swim modes (push, pull and wrap)? We use a dedicated microscopy setup to simultaneously image bacterial swimmers in bright-field and fluorescence mode in order to respectively collect time-sampled trajectories and identify their swim modes. Based on the trajectories, we analyze particle- based Langevin-type models in order to address the question of how bacteria with a given motility pattern colonize their environments, and how efficient the foraging dynamics is. In the long term, we plan to study collective pattern formation, for example, aggregation induced by inter-particle signalling. The emergent dynamics will then be described by reaction-diffusion-advection type stochastic, nonlinear partial differential equations due to the coupling of motility and particle density.

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Deutsches Elektronen-Synchrotron, DE | **Johannes Dora**

Enabling online views for holographic in-situ

Dora, J., Hagemann, J., Grosser, M., Flenner, S., Greving, I., Knopp, T., and Schroer, C.

The PETRA III Storage Ring at DESY in Hamburg is one of the world's brightest storage-ring-based X-ray radiation sources that offers a beam with a very high brilliance. It is used by researchers from all around the world to investigate small samples down to the resolution of some nanometers. Near-field holography is one of the major imaging techniques where a full-field projection is captured with a single exposure. The reconstruction of the complex refractive index of the sample from the recorded detector data is typically done during post processing and demands a high amount of manual steps and time. Exact setup parameters need to be determined, the reconstruction suffers from slow convergence and, due to the non-convex nature of the inverse problem, it is easily stuck in a local minima. The optical evaluation of the measurement results during the beam time is prevented, which makes in-situ experiments unfeasible. The purpose of this study was to investigate the impact of additional regularization terms for the cost functions as well as different treatments of the real and imaginary part of the refractive index on the reconstruction performance of the currently used algorithm. We could show empirically that local minima are already reached during the few first few hundred iterations and that the reconstruction performance significantly benefits from a strongly regularized warm-up phase as well as independent updates of the real and imaginary part of the refractive index. By using a fused lasso regularization for the warm-up phase, a sufficient reconstruction quality was achieved in a reasonable amount of time.

We where then able to build a proof-of-concept program that provides the operator with an online view of the sample at the P05 beam line.

Damien Fournier | MPI for Solar System Research, DE

Imaging large-scale flows in the Sun using time-distance helioseismology

Time-distance helioseismology measures the wave travel times between any two locations at the solar surface. From these measurements, one wants to infer internal properties of the Sun such as density, sound speed or large-scale axisymmetric flows (meridional circulation or differential rotation). The first step is to solve the forward problem which characterizes the propagation of acoustic waves in the solar interior. We use a simplified model where the divergence of the wave displacement is solution of a scalar wave equation and solve this equation using the finite element method [1]. A difficulty for solar applications is the strong variations of the background coefficients. Obtaining an accurate numerical solution requires particular care in constructing the mesh and in the derivation of atmospheric radiation boundary conditions. With the knowledge of the Green's function of the forward problem, we can compute Born sensitivity kernels which relate the measured travel times to the flows [2] and solve the inverse problem. We use the Tikhonov regularization method and show the importance of adding physical constraints such as mass conservation to obtain reliable solutions. The inversion is validated on synthetic data and applied to observations from ground- and space-based telescopes. Inversion results for the meridional flow [3] and the solar differential rotation will be presented.

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Marina García Peñaranda | GFZ, DE

Ring Current Reconstruction via Multi-Satellite Observations and Comparison with VERB-4D Reanalysis Data.

The Earth's ring current is a complex dynamic system that plays an important role in geomagnetic storms.

This ring-shaped current environment changes its struture and intensity on different time scales as a result from the incoming solar wind. Particle populations display very different behaviors, making it extremely hard to develop physics-based forecasting models for the ring current environment. Satellite data provides electron point measurements that can be used to study the different physical processes occurring in the Earth's magnetospheric ring current. However, in order to fully understand the particle dynamics and injection processes in this region, high temporal and spatial data resolutions are required. We attempt to tackle this issue by using a combination of electron-flux observations from different satellite missions and instruments, in order to improve the global resolution of this dynamic environment. In this work, we present a global reconstruction of the ring current population (energies from ~1 to a few 100 keV) using global multi-satellite data from POES, GOES, THEMIS and the Van Allen Probes (RBSP) missions. We achieved this by intercalibrating the satellite data for the year 2017. Additionally, we present a comparison of the observed electron flux environment with a reanalysis of the ring current region obtained by using the simplified version of the VERB-4D, which solves the convection equation and reduces the problem to a two-dimensional case using parameterized lifetimes τ. For the reanalysis, we assimilate GOES and Van Allen Probes (RBSP A and RBSP B) data with a Stardard Kalman Filter.

University of Potsdam, DE | **Gottfried Hastermann**

Analysis of Signal Tracking in Partially Observed Systems

Hastermann, G., and de Wiljes, J.

With large scale availability of precise real time data, their incorporation into physically based predictive models, became increasingly important. This procedure of combining the prediction and observation is called data assimilation. One especially popular algorithm of the class of Bayesian sequential data assimilation methods is the ensemble Kalman filter which successfully extends the ideas of the Kalman filter to the non-linear situation. However, in case of spatio-temporal models one regularly relies on some version of localization, to avoid spurious oscillations. In this work we develop a-priori error estimates for the time continuous variant of the ensemble Kalman filter, known as localized ensemble Kalman–Bucy filter. More specifically we aim for the scenario of sparse observations applied to models from fluid dynamics.

Fabian Hinterer | Johannes Kepler University Linz, AT

A projected Nesterov-Kaczmarz approach to stellar population-kinematic distribution reconstruction in Extragalactic Archaeology

Hinterer, F., Hubmer, S., Jethwa, P., Soodhalter, K., van de Ven, G., and Ramlau, R.

We consider the problem of reconstructing a galaxy's stellar population distribution function from spectroscopy measurements. These quantities can be connected via the single-stellar population spectrum, resulting in a very large scale integral equation with a system structure. To solve this problem, we propose a projected Nesterov-Kaczmarz reconstruction (PNKR) method, which efficiently leverages the system structure and incorporates physical prior information such as smoothness and non-negativity constraints.

Lukas Holbach| Johannes Gutenberg University Mainz, DE

Inferring Geometries and Rheological Properties of Tectonic Plates Using a Bayesian Level Set Method

Holbach, L., Gurnis, M., and Stadler, G.

To understand the movement inside the Earth, we aim to reconstruct the shape of tectonic plates and infer material properties such as density or viscosity from surface observations. Modeling lithospheric flow using incompressible instantaneous Stokes equations, the problem is formulated as an infinite-dimensional Bayesian inverse problem. Subsurface structures are described as level sets of a smooth auxiliary function, allowing for flexible topological changes. Since inverting for subsurface structures from surface observations is inherently challenging, we propose a method that incorporates prior knowledge about plate geometries stemming from seismic images into the prior probability distribution. The posterior probability distribution is explored using a Markov chain Monte Carlo method. We apply the method to a realistic model problem describing a subduction zone. The aim is to infer the geometry of the subducting plate and its density as well as the viscosity in the hinge zone. Furthermore, we investigate the effect of different data types on the inversion, comparing measurements of plate velocities, normal stresses, and their combination. We discuss the benefits and limitations of our method, show trade-offs between different parameters, and provide physical interpretations.

University of British Columbia, CA | **Brian Irwin**

Derivative Free Optimization Methods For Inverse Problems

Inverse problems formalize the relationship between experimental data and mathematical models. Estimating the parameters of the mathematical model given experimental data generally involves minimizing an objective function quantifying the misfit between the experimental data and the outputs of the forward model. When gradients of the forward model are unavailable or computationally expensive, derivative free optimization methods become attractive. Gradients of the forward model may be unavailable or difficult to compute because the components of the forward model contain non-differentiable or stochastic operations. If the forward model contains stochastic operations, exact evaluations of the objective function are not possible in general. In this work, we focus on optimization methods developed for the scenario where the gradient of the objective function is unavailable and objective function evaluations are corrupted by noise. We outline some derivative free optimization methods developed to handle the difficulties presented by this scenario.

FU Berlin, DE | **Vesa Kaarnioja**

Quasi-Monte Carlo methods for optimal control problems subject to parabolic PDE constraints under uncertainty

Guth, P. A., **Kaarnioja, V.,** Kuo, F. Y., Schillings, C., and Sloan , I. H.

Modern quasi-Monte Carlo (QMC) methods are based on tailoring specially designed cubature rules for high-dimensional integration problems. A common application within the field of uncertainty quantification is computing the statistical response of partial differential equations (PDEs) with random or uncertain coefficients. In this work, we study the application of a tailored QMC method to a class of optimal control problems subject to parabolic PDE constraints under uncertainty: the state in our setting is the solution of a parabolic PDE with a random thermal diffusion coefficient, steered by a control function. To account for the presence of uncertainty in the optimal control problem, the objective function is composed with a risk measure. We consider two risk measures, both involving high-dimensional integrals over the stochastic variables: the expected value and the (nonlinear) entropic risk measure. The high-dimensional integrals are computed numerically using QMC and, under moderate assumptions on the input random field, the error rate is shown to be essentially linear independently of the stochastic dimension of the problem - and thereby superior to ordinary Monte Carlo methods. Numerical results are presented to assess the effectiveness of our method.

Milad Karimi | University of Göttingen, DE

Towards the holographic x-ray intensity correlations: Exploring the information content

Karimi, M., and Hohage, T.

Holographic x-ray imaging enables nanoscale imaging of biological cells by exploring the phase and absorption information content of the intensity correlation data. The main difficulty of holographic x-ray imaging compared to other types of wave propagation problems is the lack of phase information since only the intensities (holograms) of the diffracted waves can be measured in the case of a partially coherent incident beam. Mathematically, a 2D-holographic x-ray imaging model is designed as an inverse problem to find the contrast function containing the phase and absorption information. In principle, the measured intensities are described by the so-called stochastic Cox-processes which are more realistic in a continuous setting. For the medium-size data sets, we have used the iteratively regularized Gauss-Newton method and error reduction method as standard iterative reconstruction methods. Surprisingly, our numerical results demonstrate that both phase and absorption contrast can jointly be reconstructed from only intensity correlations without the use of average intensities. Moreover, the quality of reconstructions gets better if only phase or absorption has to be retrieved.

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Josie König | University of Potsdam, DE

Model Order Reduction for Bayesian Inference by Balanced Truncation

The use of Bayesian inference in data assimilation provides probability distributions instead of point estimates and thus allows uncertainty quantification. Despite these quite advantageous features, one drawback is that these methods are more computationally expensive than standard approaches. Therefore, model order reduction techniques, such as balanced truncation, should be used for Bayesian inference to reduce the computational burden while maintaining accuracy. This work aims to further strengthen the connection between MOR and Bayesian inference.

University of Potsdam, DE | **Thomas Mach**

Solution of Ill-posed Problems with Chebfun

Alqahtani, A., **Mach, T**., and Reichel, L.

The analysis of linear ill-posed problems often is carried out in function spaces using tools from functional analysis. However, the numerical solution of these problems typically is computed by first discretizing the problem and then applying tools from finite-dimensional linear algebra. The present paper explores the feasibility of applying the Chebfun package to solve ill-posed problems with a regularize-first approach numerically. This allows a user to work with functions instead of vectors and with integral operators instead of matrices. The solution process therefore is much closer to the analysis of ill-posed problems than standard linear algebra-based solution methods. Furthermore, the difficult process of explicitly choosing a suitable discretization is not required.

University of Würzburg, DE | **Kristina Meth**

L^1-regularization for Inverse Problems with subexponentially-tailed data

Meth, K., and Werner, F.

Outgoing from [1] and [2] we analyze variational regularization with L^1 data fidelity. We investigate discrete models with regular data in the sense that the tails decay subexponentially. Therefore, error bounds and convergence rates are provided.

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Christian Molkenthin | University of Potsdam, DE

Bayesian earthquake forecasting

Molkenthin, C., Zöller, Z., Holschneider, M., and Hainzl, S.

Temporal dynamics of earthquake occurrence are often statistically modeled by the Epidemic type aftershock sequence (ETAS) model, which describes a self-exciting Hawkes point process. The ETAS model considers the spatio-temporal clustering of earthquakes as it is observed in nature, e.g. aftershock sequences, and it is broadly used for seismic forecasting. Calibration of the model parameters using earthquake data is usually done via maximum likelihood estimation. Uncertainty quantification and incorporation of prior knowledge remains, however, challenging. In contrast, Bayesian methods allow directly to include priors and to consider the uncertainty of the model estimates when generating forecasts. A Bayesian approach is rarely applied to the ETAS model as the evaluation of the posterior distribution is not straightforward. Markov-Chain-Monte-Carlo (MCMC) methods have to be employed. We present semiparametric Bayesian inference of the spatio-temporal ETAS model combining Hawkes point process with Gaussian process (GP) modelling. Further we use a sparse GP approximation in order to render the approach possible also for large data sets. Examples of test sites in seismic active regions illustrate the advantages of the proposed Bayesian approach.

Gregor Pasemann | Humboldt University of Berlin, DE

Diffusivity Estimation for Stochastic Parabolic Equations under Observation Noise

Pasemann, G., and Reiß, M.

We consider the problem of parametric inference for a stochastic heat equation from observations perturbed by small additive noise. We examine the tradeoff between exploiting small-scale spatial information and smoothing out the noise, and derive optimal convergence rates. In this setting, the dynamic noise and the observation noise play qualitatively different roles. (This is work in progress with Markus Reiß.)

University of Potsdam, DE | **Christian Riedel**

Research Data Management in the CRC 1294

Riedel, C., Lucke, C., and Engbert, R.

reating digital data and software code is crucial in generating scientific findings, and therefore, adequate scientific data quality and access are essential when building consecutive scientific results. To address this issue, numerous stakeholders across scientific disciplines established policies for handling and publishing research data [1, 2]. Such guidelines predominantly address open science practices and reproducible research results. However, the abundance of different guidelines mixed with individual requirements and dependencies in the research community results in a very heterogeneous picture concerning data management and data publication, which requires the scientific community's attention. At the same time, interdisciplinary guidance and support structures may be challenging to access for individual researchers. Since the beginning of its first funding period, the CRC1294 has supported associated researchers in their data management in two areas: (1) the provision of IT infrastructure to strengthen collaborative work and best practices in data handling, and (2) knowledge perpetuation by providing individual support and workshops to researchers. The support structures cover aspects throughout the research data life cycle and assist in the progress of implementing FAIR data principles and publishing reproducible scientific results. When investigating the reproducibility of scientific results, we found that the reproducibility of the CRC's publications increased over time. We attribute this development to the CRC's support structures and a general trend toward open science in many research communities. Despite this positive trend, limitations due to data accessibility and quality shortcomings indicate a continuous demand for such support structures among researchers [3]. To further support the publication of open and reproducible scientific results, the CRC shares the experiences and feedback from associated scientists with diverse stakeholders in research. Based on our experiences, we give recommendations on removing barriers to the accessibility and reproducibility of scientific findings. Recommendations to the research community include establishing institutional support structures in research data management, implementing compulsory artifact sharing and reproducibility checks, and recognizing research data as scientific achievements.

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Bernhard Stankewitz | Humboldt University of Berlin, DE

Sequential early stopping for L2-boosting in high dimensional models

In the context of increasingsly high dimensional data sets, estimation methods do not only have to provide statistical guarantees but also ensure computational feasibility. For iterative procedures, sequential early stopping can substantially reduce computational complexity, while maintaining statistical guarantees in terms of adaptivity. I present new results for L2-boosting in high dimensional models.

Maia Tienstra | University of Potsdam, DE

Frequentist EnFK

Tienstra, J., Pidstrigach, J., and Reich, S.

We are interested in the Tikhonov type regularization of statistical inverse problems. The main challenge is the choice of the regularization parameter. Hierarchical Bayesian methods and Bayesian model selection give us theoretical understanding of how the regu- larization parameters depend on the unknown data. One popular way to solve statistical inverse problems is using the Ensemble Kalman filter (EnKF). We formulate a frequentist version of the continuous time EnKF, which brings us to the well known bias and variance tradeoff of our estimator dependent upon the regularization parameter. From here we can reformulate the choice of regularization parameter as a choice of stopping time dependent on estimation of the residuals. We are currently exploring the theoretical questions that arise from the frequentist EnKF. We numerically explore this through a simple linear inverse problem, and we are further interested in its performance on non-linear inverse problems.

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NOTES

DFG Deutsche Forschungsgemeinschaft

SFB 1294 Data Assimilation

CRC 1456 MATHEMATICS OF EXPERIMENT

GIP Gesellschaft für Inverse Probleme e.V.