2nd annual Dutch Inverse Problems Meeting

Summary

Following a very successful first meeting in 2021, the second installment was organized on November 10-11 2022 in conference center *De Werelt* in Lunteren.

The goal of the workshop was to provide an opportunity for researchers working on inverse problems in various disciplines to exchange ideas, identify open problems, and form new scientific collaborations.

The program was split in two parts. On the first day, two masterclasses gave an in-depth overview of the theory of inverse problems and scientific computing. These were aimed primarily at PhD students, but were also attended by senior researchers. For the second day, we invited researchers from various disciplines to give an overview of current research surrounding inverse problems from both a theoretical and practical point of view.

The meeting was attended by ca. 45 researchers of varying seniority and background. We saw many returning participants who attended last year, and new ones as well. It is clear that both masterclasses and the broad range of research talks are appealing to many researchers in the area of inverse problems and that bringing these together across disciplines leads to many new ideas and connections. We aim to organize the meeting again next year.

The program, abstracts and an overview of the budget are included on the subsequent pages.

Group picture of participants on Friday
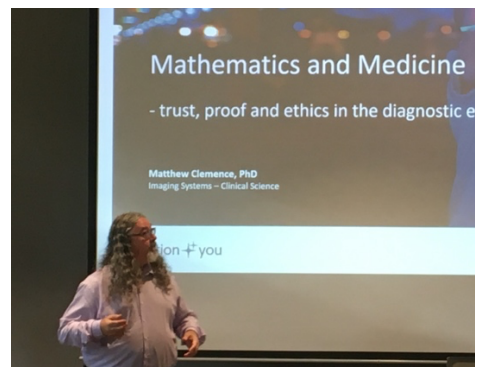
Matthew Clemence (Philips Healthcare)

Program

Thursday November 10

The masterclasses on *Inverse Problem Theory* and *High Performance Computing* aim to give an in-depth overview and hands-on experience on the topic.

09.30 - 10.00: Reception, coffee

10.00 - 13.00: **Masterclass by Tristan van Leeuwen (Centrum Wiskunde & Informatica):** *Inverse Problem Theory*

13.00 - 14.00: Lunch break

14.00 - 17.00: **Masterclass by Kees Lemmens (TU Delft):** *High Performance Computing*

17:00 - 18.00: Drinks

18:00 - 20.00: Dinner

Friday November 11 (unfortunately, we had some last-minute cancellations due to illness)

Scientific talks, highlighting recent developments in Inverse Problems from a mathematical and practical point of view. The talks are by invitation, and selected to give a balanced perspective on theory and applications of inverse problems from both junior and senior researchers.

08.45 - 09.15: Reception, coffee

09.15 - 10.00: **Plenary lecture by Carola Bibiane Schönlieb (University of Cambridge):** *Data-driven regularisation for solving inverse problems*

10.00 - 10.30: Coffee break Reception, coffee

10.30 - 12.00: **Olga Mula (TU Eindhoven):** *Optimal State and Parameter Estimation Algorithms and Applications to Biomedical Problems*
Alessandro Sbrizzi (UMC Utrecht): *Fast Quantitative MRI as a large scale ODE constrained problem: MR-STAT*
Julia Engelmann (NIOZ): *Predicting marine microbial interactions with causal discovery*

12.00 - 13.30: Lunch break

13.30 - 14.30: **Christoph Brune (University of Twente):** *Geometric Deep Learning for Dynamic Inverse Problems*
Ronald Quirchmayr: *Inverse scattering and asymptotics for the defocusing nonlinear Schrödinger equation*

14.30 - 15.15: **Plenary lecture by Matthew Clemence (Philips Healthcare):** *Mathematics and Medicine – trust, proof and ethics in the   diagnostic environment*

15.15 - 15.45: Coffee break

15.45 - 16.15: **Palina Salanevich (University of Utrecht)** *Stability of phase retrieval with Gabor measurements*

15.45 - 16.15: **Felix Lucka (CWI)** *Photoacoustic and Ultrasonic Tomography for Breast Imaging*

16:15 - 17.30: Drinks

Abstracts

Inverse Problem Theory (Tristan van Leeuwen - CWI)

There is a rich mathematical theory behind inverse problems, which can be very useful in practical applications. This masterclass covers the basics of inverse problem theory, including:

- Ill-posedness and regularisation
- Bayesian modelling
- Optimisation-based solution strategies
- Uncertainty quantification

In the first part, we treat these concepts in detail for linear, discrete inverse problems and point out the broader context using practical examples. We will also get some hands-on experience with the concepts using Python. In the second part you are encouraged to discuss how the concepts apply to your own research in small groups.

As a prerequisite, we expect basic knowledge of linear algebra (including singular value decomposition), calculus, least-squares problems, and basic statistics (i.e., Gaussian distributions). Knowledge of Python or Matlab (and a laptop) will come in handy.

High Performance Computing (Kees Lemmens - TU Delft)

Mathematicians and engineers sooner or later will have to convert their ideas and formulas into computer code, for instance, if they want to run a simulation. At that point, many decide to sort of learning a little programming in a 60 minutes online crash course (e.g., using Matlab), start to do their coding, and are already quite happy if the program seems to produce some output without too many error messages. But while coding they often make several very common and basic errors without realizing this, which may occasionally cause very strange results. So, the most fundamental thing I want you to learn during this course is: "Do not trust either a computer or an algorithm blindly!" Another important aspect is computational efficiency; you don't want to wait for a result for 1 week if it can be done in an hour! A possible solution to this is Parallel Computing, but this comes with its own challenges to get it right. We treat the following topics;

- basic usage of Linux, Python, C, and useful libraries for mathematics
- floating-point arithmetic; overflow, underflow and catastrophic cancellation
- writing efficient code
- parallel computing (scalability, speedup, deadlocks and race conditions)
- high-performance computing using GPUs

Although not required it may help if you have some (very) basic knowledge of C and/or Python. You won't believe it but even Matlab knowledge may already help (a little ;-)) and of course, some basic knowledge of mathematics doesn't hurt as well! The part on Parallel and High-Performance Computing shouldn't require any other prior knowledge apart from what is mentioned above.

Data-driven regularisation for solving inverse problems (Carola Bibiane Schönlieb, University of Cambridge)

Most inverse problems of interest are ill-posed and require appropriate mathematical treatment for recovering meaningful solutions. Regularization is one of the main mechanisms to turn inverse problems into well-posed ones by adding prior information about the unknown quantity to the problem, often in the form of assumed regularity of solutions. Classically, such regularization approaches are handcrafted. Examples include Tikhonov regularization, the total variation and several sparsity-promoting regularizers such as the L1 norm of Wavelet coefficients of the solution. While such handcrafted approaches deliver mathematically and computationally robust solutions to inverse problems, providing a universal approach to their solution, they are also limited by our ability to model solution properties and to realise these regularization approaches computationally. Recently, a new paradigm has been introduced to the regularization of inverse problems, which derives regularization approaches for inverse problems in a data driven way. Here, regularization is not mathematically modelled in the classical sense, but modelled by highly over-parametrised models, typically deep neural networks, that are adapted to the inverse problems at hand by appropriately selected (and usually plenty of) training data.

In this talk, I will review some machine learning based regularization techniques, present some work on unsupervised and deeply learned convex regularisers and their application to image reconstruction from tomographic and blurred measurements, and finish by discussing some open mathematical problems.

Optimal State and Parameter Estimation Algorithms and Applications to Biomedical Problems (Olga Mula, TU Eindhoven)

In this talk, I will present an overview of recent works aiming at solving inverse problems (state and parameter estimation) by combining optimally measurement observations and parametrized PDE models. After defining a notion of optimal performance in terms of the smallest possible reconstruction error that any reconstruction algorithm can achieve, I will present practical numerical algorithms based on nonlinear reduced models for which we can prove that they can deliver a performance close to optimal. The proposed concepts may be viewed as exploring alternatives to Bayesian inversion in favor of more deterministic notions of accuracy quantification. I will illustrate the performance of the approach on simple benchmark examples and we will also discuss applications of the methodology to biomedical problems which are challenging due to shape variability.

Fast Quantitative MRI as a large scale ODE constrained problem: MR-STAT (Alessandro Sbrizzi, UMC Utrecht)

Conventional quantitative Magnetic Resonance Imaging (qMRI) is based on a two steps approach, namely: (1) transformation from k-space to image domain and (2) voxel-by-voxel estimation of quantitative MR parameters. Magnetic Resonance Spin-TomogrAphy in Time-domain (MR-STAT) is a recently proposed technique where these two steps are simultaneously performed by casting the reconstruction process as a single, large-scale non-linear inverse problem. As a consequence, standard constraints on the acquisition protocol can be relaxed and the duration of the scan drastically shortened. Results from the first MR-STAT clinical trial show that a full-brain multi-slice protocol of 5 minutes can successfully return multi-parametric maps at 1 mm2 in-plane resolution. In this talk, I will illustrate the potentials and the challenges of the MR-STAT approach which include: numerical complexity, efficient solutions of the underlying time-dependent ODE, approximation of the Hessian during the optimization process, noise propagation, experimental design, issues of convexity etc.

Predicting marine microbial interactions with causal discovery (Julia Engelmann, NIOZ)

Microorganisms form the base of the marine food web. While phytoplankton use inorganic carbon and sunlight to generate carbohydrates and oxygen, they are consumed by zooplankton which again are consumed by increasingly larger animals. Bacteria and viruses decompose organic material and make nutrients available again. While we understand these processes from a bird's-eye view, the intricate interplay between different microbial species is still mostly hidden. This is due to the huge amount of different microorganisms and potential interactions, and the fact that pairwise interactions between microorganisms are difficult to study experimentally. The majority of marine microorganisms cannot be cultured in a laboratory, which also indicates that species-species interactions are crucial for marine microorganisms to thrive. I will show how we use causal discovery to predict marine microbial interactions from observational abundance data. We first derive microbial abundance from sequencing DNA of cells extracted from seawater. Multiple abundance profiles over space or time serve as input to reconstruct Bayesian networks, which can then be queried for causal effects one microbial species might have on the abundance of another microbial species. This allows us to come up with a smaller set of potential interaction hypotheses to follow up with.

Geometric Deep Learning for Dynamic Inverse Problems (Christoph Brune, University of Twente)

For inverse problems in imaging the combination of model-driven and data-driven approaches evolved as a strong paradigm for scientific innovation. Recently, geometric deep learning exploring model geometry (reduction and symmetry) and data geometry (reduction and representation) quickly gained attention in science. In particular, graph neural networks, physics-informed neural networks and deep kernel learning for model reduction arose as key techniques. This talk will focus on time-dependent inverse problems and highlight examples of those key techniques for improved model exploration, model reduction and uncertainty quantification. 4D medical imaging and reinforcement learning for digital twins illustrate the potential impact.

Inverse scattering and asymptotics for the defocusing nonlinear Schrödinger equation (Ronald Quirchmayr, University of Vienna)

We present results concerning the Cauchy problem for the defocusing nonlinear Schrödinger equation under the assumption that the solution vanishes as x goes to positive infinity and approaches an oscillatory plane wave as x goes to negative infinity. This talk covers the corresponding direct and inverse scattering transform via a Riemann-Hilbert formalism, the existence of a global solution for the Cauchy problem and the derivation of its long-time behavior by means of a steepest descent analysis.

Mathematics and Medicine – trust, proof and ethics in the diagnostic environment (Matthew Clemence, Philips Healthcare)

The development of Magnetic Resonance Imaging has been driven by advances in computing, signal processing and image processing methods. Mathematical methods touch all aspects of image production and the generation of quantitative data to guide the physician to both successful diagnosis and treatment guidance. In recent years, increasing usage of mathematical modelling and deep learning methods are being applied to address the problems of workflow, capacity and cost which are challenging healthcare institutions around the world. However these techniques are raising new challenges of medical ethics, public acceptance and regulatory. This presentation will briefly outline the basics of MRI image production, and the applications, and landscape for the challenges for the deployment of these methods in healthcare.

Stability of phase retrieval with Gabor measurements (Palina Salanevich, University of Utrecht)

Phase retrieval is the non-convex inverse problem, where we aim to recover a signal from its intensity measurements with respect to a frame of measurement vectors. This problem arises in many practical applications, such as diffraction imaging, audio processing, radars, and many more. Even though it has been studied for a long time, until recently very little was known about how to achieve stable and efficient reconstruction, and the existing reconstruction methods lacked rigorous mathematical understanding. Nowadays, the case when the measurement frame is a Gaussian frame with independent frame vectors is sufficiently well studied. At the same time, very little is known about the case of structured, application relevant frames. One of the main reasons for this is that geometric properties of such structured frames are not yet fully understood.
In the talk, we are going to focus of the Gabor frames, where the measurement vectors are obtained by time-frequency shift of a Gabor window. Such frames naturally appear in imaging and acoustic applications. We will overview the recent developments on the stability of phase retrieval with Gabor measurements and the arising open questions and challenges. We will also discuss the link between geometric properties of frames, such as frame order statistics , reflecting how "flat" the vector of frame coefficients can be, and stability of the phase retrieval problem.

Photoacoustic and Ultrasonic Tomography for Breast Imaging (Felix Lucka - CWI)

New high-resolution, three-dimensional imaging techniques are being developed that probe the breast without delivering harmful radiation. In particular photo-acoustic tomography (PAT) and ultrasound computed tomography (USCT) promise to give access to high-quality images of tissue parameters with important diagnostic value. However, the involved image reconstruction problems are very challenging from an experimental, mathematical and computational perspective. In this talk, we want to illustrate some of these challenges with data from an ongoing clinical feasibility study that uses a prototype scanner for combined PAT and USCT. In particular, we will discuss Full Waveform Inversion (FWI) approaches for speed-of-sound imaging with USCT and iterative model-based reconstruction approaches for PAT. To obtain high-quality 3D images with 0.5mm resolution or less, PDEs modeling ultrasound propagation through domains with different material properties needs to be solved repeatedly and to a high accuracy. After reviewing our current results, we will discuss future developments that will broaden the range of clinical scenarios in which these techniques are viable.

Budget

Description	In	Out
Total costs De Werelt		13000
Registration fees	6000	
NWO	2250	
CWI-CI	1125	
NDNS+	1000	
DIAM	2000	
Bernoulli	750	
Total	**13125**	**13000**