NEWSLETTER ISSUE 1

Welcome to Maths4DL

The £3.5M EPSRC Programme Grant on the Mathematics of Deep Learning, (Maths4DL) awarded to the University of Bath, University of Cambridge and University College London, commenced in February 2022.

The Mathematics of Deep Learning (Maths4DL) programme aims to put deep learning onto a firm mathematical basis, and will combine theory, modelling, data and computation to unlock the next generation of deep learning.

The research aims to address both the theoretical development of DL (so that it becomes explainable) and the algorithmic development (so that it becomes trustworthy). These will then be linked to the development of DL in a number of key application areas, linked to and supported by industry, including medical image processing, partial differential equations and environmental problems.

Meet the Team

The steering committee has expertise in many areas of deep learning, including interdisciplinary mathematics, statistics, Artificial Intelligence (AI), Partial Differential Equations (PDEs), optimal transport, optimisation, environmental modelling, numerical analysis, geometric integration, scientific computing, image processing, probability, and inverse problems.

The Team also has extensive research networks and strong links with major research centres and other external partners. These contacts have already been put to good use in the work carried out so far and this began with the opening workshop which attracted many of our partners.

Investigators:
Simon Arridge (UCL)
Chris Budd OBE (Bath)
Matthias Ehrhardt (Bath)
Bangti Jin (UCL)
Richard Nickl (Cambridge)
Carola-Bibiane Schönlieb (Cambridge)

Domain Experts:
Tatiana Bubba (Bath)
Yury Korolev (Bath)
Lisa Kreusser (Bath)

Post Doctoral Research Associates:
Kweku Abraham (Cambridge)
Teo Deveney (Bath)
Rob Tovey (UCL)
Hok Shing Wong (Bath)

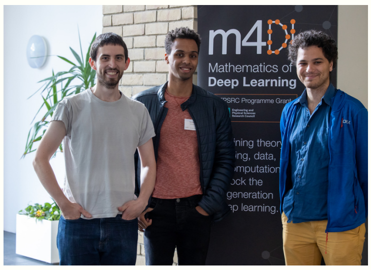
Programme Manager
Helena Lake (Bath)

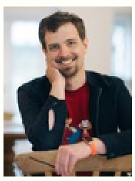
Recruitment

We welcomed Rob Tovey to the team as PDRA at UCL in September and we have recruited our second PDRA in Bath. We look forward to working with Hok Shing who starts in late November.

Yolanne Lee began her Maths4DL PhD studentship at UCL in September.

Yury Korolev has joined the University of Bath as Lecturer.





Opening workshop 21-22 April 2022

https://people.bath.ac.uk/td314/m4dlworkshop/m4dl-workshop.html

The launch event for Maths4DL took place in Bath in late April and saw students, academics and industry get together to hear some fascinating talks from, among others, several of our external advisory board members.

The workshop included talks from Andrew Fitzgibbon (Graphcore), Kweku Abraham and Subhadip Mukherjee from Cambridge, Riccardo Barbano (UCL), Teo Deveney and Lisa Kreusser from Bath, Gitta Kutyniok (LMU), and Kwinten van Weverberg from the Met Office. On the second day of the workshop we heard from Jong Chul Ye (KAIST), Keith Briggs (BT), Weinan E (Princeton), Sandeep Kaushik, Carolin Pirkl and Timo Schirmer from GE Healthcare as well as Margaret Duff (Bath) and Yury Korolev (Cambridge). The workshop ended with an open discussion where all attendees had a chance to put forward their thoughts on the challenges of deep learning.



Maths4DL sponsored events in 2022

Statistical Learning and Differential Privacy, 12-13 September at Bath

https://mathematics-and-algorithms-for-data.github.io/events/workshop_SLDP2022/

LMS Analytic and Geometric Approaches to Machine Learning, 11-15 July, 2022 at Bath.

https://bathsymposium.ac.uk/symposium/analytic-and-geometric-approaches-to-machine-learning/

Deep learning for environmental problems 20-21 September at Bath

https://people.bath.ac.uk/td314/envdl/envDL.html



Maths4DL research

Physics-Based Neural Networks

Due to their unprecedented expressivity in high-dimensional spaces, deep neural networks have emerged as powerful ansatz functions for approximating partial differential equations (PDEs). A large variety of techniques have been developed in recent years, among which the most prominent ones include physics informed neural networks and deep Ritz method.

The team has been exploring the use of deep Ritz method for challenging direct and inverse problems for PDEs. One particularly challenging class of problems for neural network based PDE solvers is to deal with problems with low regularity problem data, e.g., singular sources, discontinuous coefficients and nonsmooth domains. One approach to tackle the outstanding challenge is to build physical and mathematical insights into the construction of neural network-based solvers. For example, in the singularity reconstruction deep Ritz method [2], one splits the solution into a singular part and a regular part, and only approximates the latter using neural networks. This method has been shown to be highly effective for problems with singular sources, cf. Fig. 1.

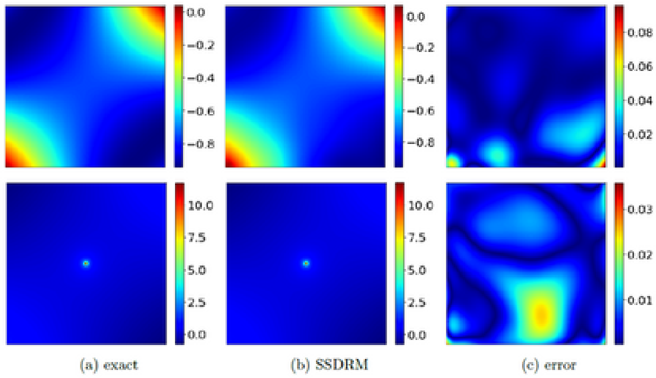


Fig. 1: neural network approximation for 3D PDE with line sources [2].

Meanwhile, the implicit bias of deep neural networks towards smooth functions can be exploited to the advantages for solving inverse problems, e.g., in constructing approximation in the presence of severe data noise; see Fig 2 for an illustration on current density impedance imaging.

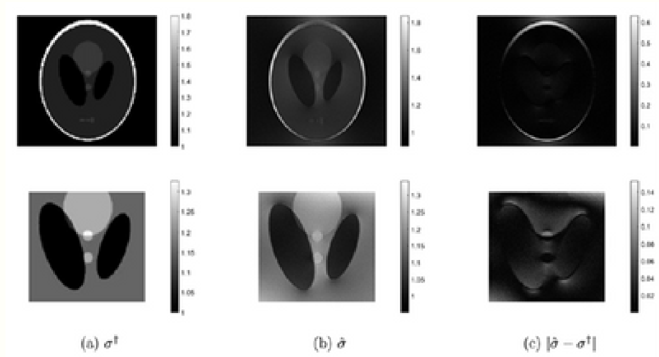


Fig. 2. Neural network reconstruction for current density impedance imaging [1].

We have also continued investigating learned solvers for Helmholtz and Maxwell's equations. The approach here is to use a recurrent neural network (RNN) including a Physics-Loss term. The application is for transcranial ultrasound (tomography and stimulation) which involves heterogeneous sound speed and/or acoustic attenuation. An example from [3] is shown in Fig.3

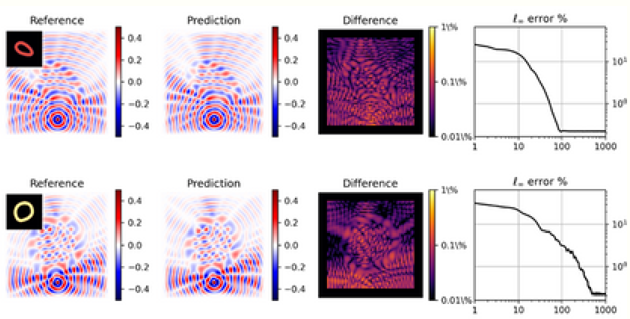


Fig. 3. Comparison of GMRes solution with learned RNN reconstruction for propagation ultrasound field [3].

The same approach has been developed for Maxwell's equations in order to model the forward problem in Optical Coherence Tomography, with comparable performance.

Maths4DL research

Uncertainty quantification for deep learning

Deep learning techniques have demonstrated astounding empirical performance on many imaging tasks. Nonetheless the techniques can mostly provide point estimators, without any information about their reliability. To empower the reconstructions with uncertainty information, Bayesian neural networks have been suggested as a principled paradigm. Nonetheless their computational complexity has hindered the widespread adoption. The team is exploring scalable uncertainty quantification in the context of deep image prior, one popular unsupervised deep learning technique. We construct uncertainty estimates using the linearized model of deep image prior, in order to adaptively incorporate the prior knowledge and building on a kernel for prior covariance in order to facilitate the computation for realistic tomographic imaging tasks. The approach shows well calibrated uncertainty estimates cf. Fig. 4, and promises extension o adaptive optimal experimental design in simulated study in Fig, 5.

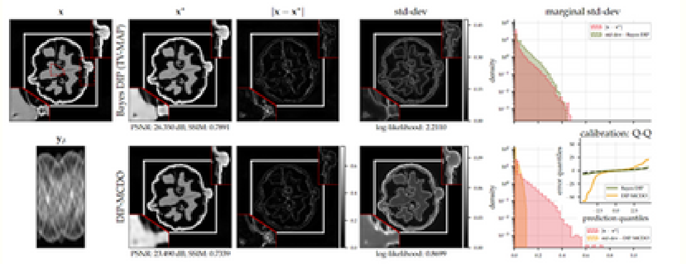


Fig. 4: probabilistic deep image prior for computed tomography on the walnut dataset [1]

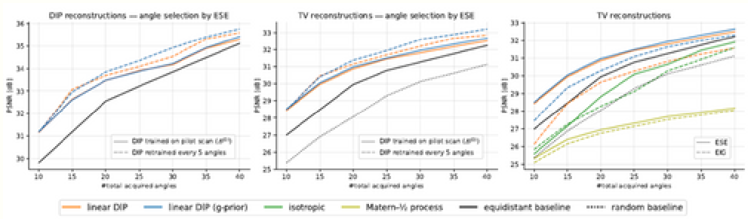


Fig. 5: experimental design with probabilistic deep image prior on synthetic data [2]

Learned Approximate Models

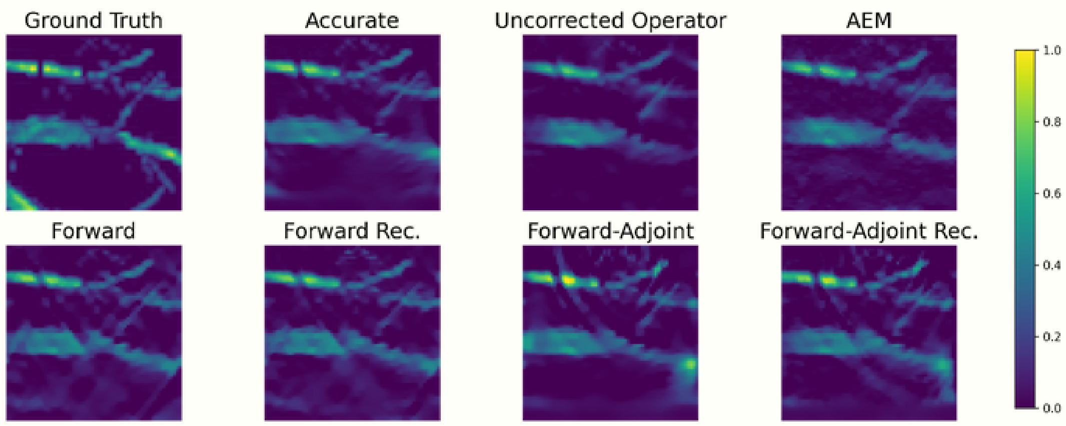
We are interested in the general idea of forward and inverse mappings between spaces X and Y which combine learning with domain specific Physics based models. We thus consider models of the form

Aq : X -> Y = Fq ÃHf

where Fq : Y -> Y is a learned mapping in data space, Hf : X -> X is a learned mapping in image space, and Ã : X->Y is an approximate forward mapping. The corresponding (linearised) adjoint mapping is then

A'*q : Y -> X = H'*f Ã'* F'*q

The use of a fast approximate mapping Ã reduces both the training (allowing end-to-end networks) and inference time for both problems. This approach was applied in [1] to PhotoAcoustic Tomography (PAT) where the approximate forward model was a Fourier regridding method with a singularity that leads to artefacts that corrected by the learned operators.



Maths4DL research

Environmental Problems

Work has got under way with the Met Office, with research also linked to WP 1.2 (PINNS).
Teo has been investigating methods of constructing deep learning models that are constrained by their architecture to preserve conserved quantities. These techniques are being applied to learn and predict the evolution of dynamical systems.

Other research work at Bath of direct relevance to Maths4DL has been (i) development, and analysis, of deep Ritz methods applied to PDEs in non-convex domains (which involved using Optimal Transport), (ii) improving realisable optimal functional approximation in deep learning using improved loss functions, (iv) using learned methods for moving mesh generation. Also work with a PhD student on deep learning for ensemble forecasting of space weather, joint with the Met Office and of direct relevance to WP 3.2

Inverse Problems in Imaging

Deep neural network approaches to inverse imaging problems have produced impressive results in the last few years, but most are lacking theoretical foundations. In parallel the machine learning community has developed powerful generative models (like VAEs and GANs) which are able to generate realistic structures, see figure. This project at Bath considers the use of generative models in a variational regularisation approach to inverse problems. The considered regularisers penalise images that are far from the range of a generative model that has learned to produce images similar to a training dataset. Thus, we call them “generative regularisers”. This approach naturally combines state-of-the-art machine learning in a theoretically sound framework for solving inverse problems.

Structure preserving deep learning

Over the past few years, deep learning has risen to the foreground as a topic of massive interest, mainly as a result of successes obtained in solving large-scale image processing tasks. There are multiple challenging mathematical problems involved in applying deep learning: most deep learning methods require the solution of hard optimisation problems, and a good understanding of the trade-off between computational effort, amount of data and model complexity is required to successfully design a deep learning approach for a given problem. A large amount of progress made in deep learning has been based on heuristic explorations. Here we aim to mathematically understand the structure in existing deep learning methods and to systematically design new deep learning methods to preserve certain types of structure in deep learning. For example, some deep neural networks can be understood as discretisations of dynamical systems and other neural networks can be designed to have desirable properties such as invertibility or group equivariance.

Uncertainty Quantification for Deep Learning

Progress is ongoing with deep gaussian processes: the adaptation question (can the deep GP prior automatically pick up structure in the signal that a standard GP would miss) is a challenging one but important if we want to advocate the merits of the deep approach.

The math-stat-appli conference in Frejus has been a highlight, where Richard Nickl presented an overview of the Bayesian approach to PDE inverse problems, culminating in his recent impossibility result for certain MCMC calculations, while Kweku enjoyed meeting Jakiw Pidstragich and discussing score-based diffusions.

Two PhD students have been working on score based diffusion idea, in the context of conditional image generation. Multi speed diffusion – e.g. used for multi scale processing of images. Also, there has been work with a PhD student on quasi linear Schrodinger equation (PINNS) and combined spectral / deep learning method to solve it.

Publications and pre-prints

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http://jmlr.org/papers/v23/20-316.html

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M Duff, I JA Simpson, M J Ehrhardt, N DF Campbell. **Compressed Sensing MRI Reconstruction Regularized by VAEs with Structured Image Covariance**
arXiv preprint arXiv:2210.14586

We've been visiting

Kweku Abraham and Bangti Jin have both had extended visits to Bath.

Matthias Ehrhardt and Lisa Kreusser presented at the Synergies between Data Science and PDE Analysis at Bonn 13-16th June 2022.

Chris Budd and Lisa Kreusser attended SciCADE at Rejkavik 25-29 July 2022.

Chris Budd spoke on deep Ritz methods in a number of seminars including the OneWorld seminar series.

Richard Nickl and Kweku Abraham attended the StatMathAppli in Frejus, France where Richard presented an overview of the Bayesian approach to PDE inverse problems.

Chris Budd spoke at the Third Symposium on Machine Learning and Dynamical Systems in Toronto in September and made good contacts with the Fields Institute as a result.

Outreach and training

Teo and Chris (together with one of Chris's PhD students, Tina Zhou), attended the Festival of Books family day at the The British Library at the end of September - demonstrating maths and puzzles to young people, including families with D/ deaf children, parents and carers.

Plus magazine

We are employing the team from the Plus magazine (based in Cambridge) to work with Maths4DL in publicising its work, and also in training all of the team in creativity. The Plus team will start by interviewing the PDRAs for podcasts, and also in writing up the environmental workshop held in September. They will then follow this up with a series of popular articles for Plus.

Awards

Congratulations to Chris Budd on receiving the SPI-M-O award for Modelling and Data Support in recognition of an exceptional contribution to the work of the Scientific Pandemic Influenza Group on Modelling (SPI-M-O).

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