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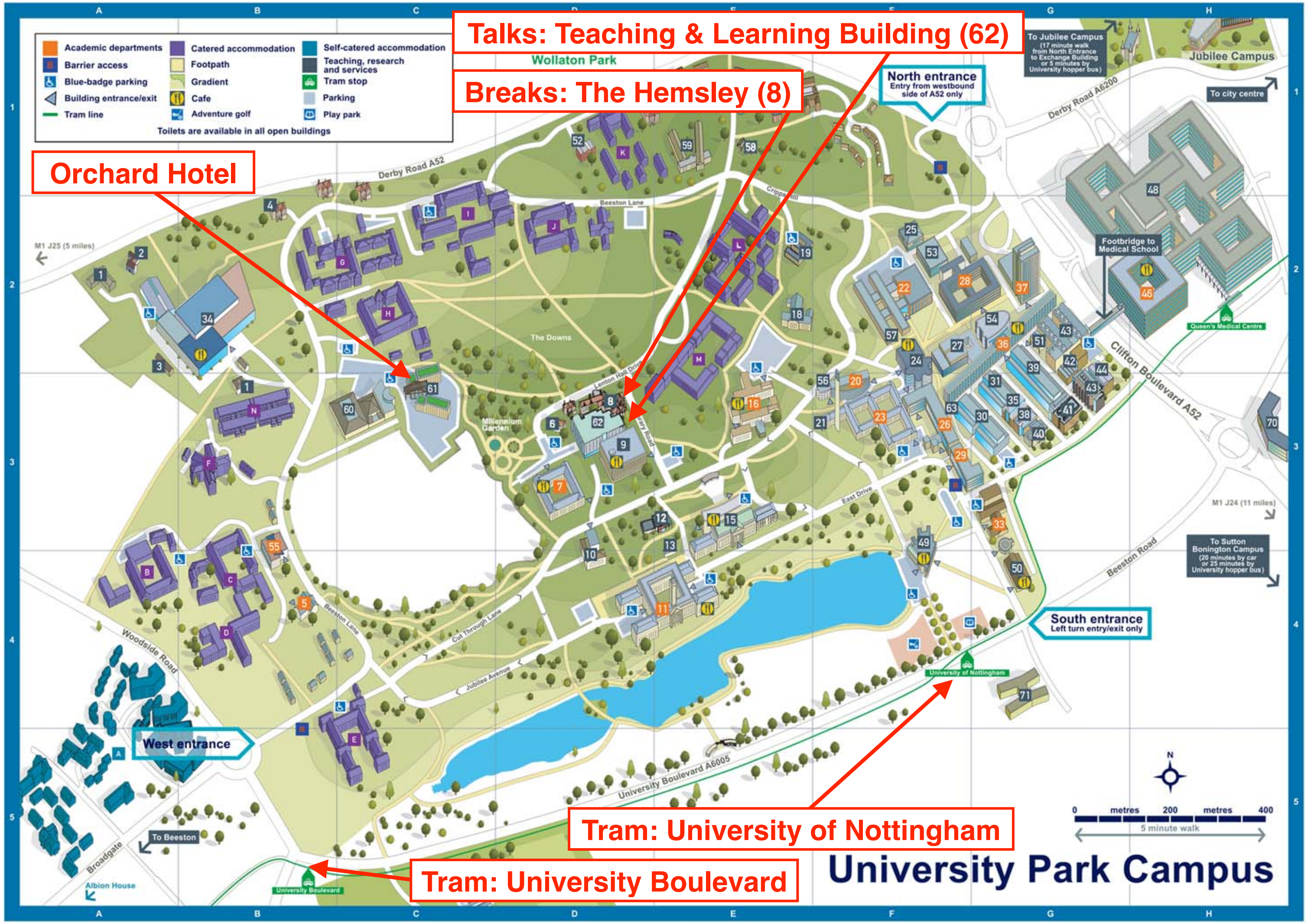
UNIVERSITY OF BIRMINGHAM

Scientific Computation using Machine-Learning Algorithms

Date: 25th and 26th April 2019

Venue: University Park, University of Nottingham



University Park campus key

Buildings in alphabetical order (and grid refrences)

Arts Centre Department of Music (G3)	33
Built Env Centre for 3D Design (D3)	58
Busy Bees Nursery (A2)	1
Centre for Biomolecular Sciences (G3)	43
Chemistry Building (F2)	28
Cherry Tree Lodge (E3)	13
Coates Building (G3)	36
Coates Road Auditorium (G2)	51
Cripps Building (E2)	19
Cripps Health Centre (E1)	59
Cripps North Building (F2)	25
Cripps South Building (F2)	53
D H Lawrence Centre (G4)	49
David Ross Sports Village (B2)	34
Day Nursery (B3)	3
East Midlands Conference Centre (EMCC) (C3)	60
Engineering and Science Learning Centre (ESLC) (G2)	54
Environmental Education Centre (E1)	14
Estates Office (F3)	21
Gatehouse Lodge (H1)	60
George Green Library (F2)	24
Hallward Library (D3)	9
Highfield House (D4)	10
Highfields Pavilion (D4)	47
Humanities (B3)	55
Institute of Hearing Research (G3)	40
Innovative Technology Research Centre (G3)	38
Keighton Auditorium (F3)	56
L2 Laboratories (G2)	39
L3 Laboratories (G3)	31
L4 Laboratories (G4)	30
Law & Social Sciences Building (D3)	7
Lenton Eaves (UNSSC Club) (B2)	4
Lenton Fields - Play Centre (A2)	1
Lenton Firs Main Bldg (E1)	17
Lenton Grove (B4)	5
Lenton Hurst (D1)	52
Lenton Lodge (A2)	2
Life Sciences (F3)	23
Manufacturing Engineering Building (G2)	42
Marmont Centre (E1)	17
Mathematical Sciences (F3)	20
Medical School (H2)	46
New Theatre (E3)	12
Nottingham Lakeside Arts (F3/G4)	49 50
NUAST (H3)	70
Orchard Hotel (C3)	61
Paton Cottage/The Stables Annexe (E1)	14
Paton House (E1)	17
Pavement Research Building (G3)	35
Pharmacy (F3)	26
Physics Building (F2)	22
Pope Building (F2)	27
Portland Building (E3)	15
Psychology (F3)	29
Queens Medical Centre (QMC) (H2)	48
Safety Office (E3)	63
Security (E3)	64
Sir Clive Granger Building (E3)	16
Sir Peter Mansfield MRI Building (E2)	18
Sustainable Research Bldg (E1)	17
Teaching and Learning Building (D3)	62
The Boots Science Building (G3)	44
The Hemsley - Lenton Mount (D3)	8
The Orchards (D3)	6
The Vaughan Parry Williams Pavilion (C5)	47
Tower (G2)	37
Trent Building (E4)	11
University of Nottingham International College	71
Wolfson Building (G30)	41
Workshop/Z Block - Built Env (E1)	17

Residential (and grid refrences)

Ancaster Hall (A4)	B
Beeston Hall (B3)	N
Broadgate Park (A4)	A
Cavendish Hall (B4)	C
Cripps Hall (E2)	L
Derby Hall (C2)	I
Florence Boot Hall (C5)	E
Hugh Stewart Hall (E2)	M
Lenton and Wortley Hall (D1)	K
Lincoln Hall (D2)	J
Nightingale Hall (B3)	F
Rutland Hall (C2)	H
Sherwood Hall (C2)	G
Willoughby Hall (B4)	D

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TEF Gold

Scientific computation using machine-learning algorithms: recent mathematical advances and applications

Over the last decade machine-learning and neural-network methodologies have matured tremendously in the areas of computer vision, language processing and data science, and have given rise to highly innovative and efficient algorithms for a wide-range of data-intensive applications.

Theoretical understanding of this remarkable performance of machine learning methodologies is an emerging topic in mathematical research. On the other hand, it has been recognised only recently that these learning methodologies lead to new solution paradigms for the computational applied sciences, with significantly more efficient algorithms and the potential to cause a step change in designing solution techniques for large-scale problems.

The aim of this workshop is to discuss recent advances in mathematical foundations of machine learning and artificial neural networks as well as the application of these methodologies in computational science.

Venue

The workshop will take place on University Park Campus at the University of Nottingham.

Key buildings (with their numbers on the campus map, see previous page):
Talks: Teaching and Learning Building (62), Room C14
Breaks / Lunches: The Hemsley (8)

Registration will take place in Teaching and Learning Building (62) from 9.15am until 9.50am on Thursday 25th April.

Talks will take place in the Teaching and Learning Building (62), Room C14.

Local transportation (tram, bus, taxi)

University Park Campus is a large campus that is well connected by tram, bus and accessible by taxis. Two convenient tram stops are “University of Nottingham” and “University Boulevard” which connect to the Nottingham city center (e.g., “Old Market Square” and “Nottingham Station”). For buses see https://www.nottingham.ac.uk/sustainability/transport/publictransport/busservices.aspx. Good taxi services include “DG Cars” (+44 115 9 500 500) and “Uber”.

Coffee breaks and lunches

Coffee/tea, refreshments and lunches will be provided at the times indicated in the programme in The Hemsley (which is the building next to the Teaching and Learning Building).

Dinner on Thursday

We will go out for dinner on Thursday evening to the restaurant MemSaab in Nottingham city centre. Further details will be communicated on the day.

Internet Access

Visiting delegates can access the University WiFi in one of two ways:
1. **Eduroam.** Connect to Eduroam as you would at your home institution. You may need to forget Eduroam and connect to it as intended. Additional guidance on
https://www.nottingham.ac.uk/it-services/connect/wifi/academics.aspx

2. **UoN-guest network.** There is the UoN-guest network for short term visitors including conference delegates. Connect to UoN-guest and create an account (which needs confirmation through email). Additional guidance on https://www.nottingham.ac.uk/it-services/connect/wifi/visitors.aspx

Acknowledgement

The organisers would like to thank the Universities of Birmingham and Nottingham for financial support of the workshop through the Birmingham–Nottingham Strategic Collaboration Fund.

Programme

Thursday 25th April 2019

09.15 – 09.50	Registration
09.50 – 10.00	Welcome and opening remarks
10.00 – 11.00	**Jan Hesthaven** *On the Use of Machine Learning in Computational Science and Engineering*
11.00 – 12.00	**Philipp Petersen** *Challenges and Opportunities for Numerical Solvers of PDEs Based on Deep Neural Networks*
12.00 – 13.30	Lunch
13.30 – 14.30	**Jakub Marecek** *Scaling Up Deep Learning for PDE-based Models*
14.30 – 15.30	**Kaj Nyström** *Some Thoughts on Neural Networks, PDEs and Data-Driven Discovery*
15.30 – 16.10	Coffee break
16.10 – 16.35	**Markus Geveler** *Machine Learning Approaches for the Acceleration of the Linear Solver in PDE Simulations*
16.35 – 17.00	**Jim Magiera** *Constraint-Aware Neural Networks for Riemann Problems*
17.00 – 17.25	**Yufei Zhang** *Rectified Deep Neural Networks Overcome the Curse of Dimensionality for Nonsmooth Value Functions in Zero-Sum Games of Nonlinear Stiff Systems*

Friday 26th April 2019

09.00 – 10.00	**Martin Eigel** *A Statistical Learning Approach for Parametric PDEs*
10.00 – 11.00	**Ahmed Elsheikh** *Machine Learning Approaches for Uncertainty Quantification of Subsurface Flow Models*
11.00 – 11.40	Coffee break
11.40 – 12.40	**Desmond Higham** *Numerical Precision in Deep Learning*
12.40 – 13.30	**Panel Discussion** *Perspectives of Machine Learning Algorithms in Numerical Analysis and Scientific Computing* Panelists: **Jan Hesthaven**, **Desmond Higham**
13.30	Closing remarks and lunch

A statistical learning approach for parametric PDEs

Martin Eigel

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Parametric PDEs (as encountered in the popular field of Uncertainty Quantification) are computationally complex due to the high dimensionality of the models describing random data. Common numerical approaches are Monte Carlo methods for statistical quantities of interest and functional approximations, representing the entire solution manifold in some function space. Assuming sufficient regularity (or sparsity), the latter attain high theoretical convergence rates. In practice, this can be realised e.g. by employing some kind of (a posteriori) error control. However, the implementation usually is non-trivial and does not generalise easily.

We examine a non-intrusive Variational Monte Carlo (VMC) method based on statistical learning theory. This provides a combination of deterministic and statistical convergence results. The Galerkin solution can be computed with high probability by using a tensor recovery algorithm on a training set of generated solution realisations. Similarly, a residual a posteriori error estimator can be reconstructed easily, steering all discretisation parameters.

Machine learning approaches for uncertainty quantification of subsurface flow models

Ahmed H. Elsheikh
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Computational models for multi-phase flow in porous media relies on a number of subsurface parameters that are poorly known (e.g. porosity and permeability fields). In practical setting, these parameters are observed at sparse set of points (e.g wells) and/or indirectly using low resolution imaging techniques (seismic surveys). Quantifying the impact of these parameters on the model outputs is an important task for robust decision support and risk assessment. In this talk, I will present two different techniques to handle this challenging uncertainty propagation task given the high dimensionality of the input parameter space and the non-polynomial nonlinearities in the subsurface flow model.

In the first part of my talk, I will introduced a machine learning based multiscale method [1] for solving elliptic equations (e.g. pressure equation in subsurface flow problems). Several multiscale methods account for sub-grid scale heterogeneities using coarse scale basis functions for upscalling. For example, in the Multiscale Finite Volume method (FVM), coarse scale basis functions are obtained by solving a set of local problems over a dual-grid. In this work, we introduce a data-driven approach for estimating the coarse scale basis functions using a neural network (NN) predictor fitted using a set of training data. For uncertainty propagation tasks, the trained NN learns to generate basis functions at a lower computational cost when compared to solving the local problems. The computational advantage of this approach is realized when a large number of realizations has to be evaluated. We attribute the ability to learn these basis functions to the modularity of the local problems and the redundancy of the permeability patches between samples. The proposed method is evaluated on single phase flow problems yielding very promising results.

In the second part of my talk, I will introduce a deep residual recurrent neural network (DR–RNN) as an efficient model reduction technique for subsurface multi-phase flow problems [2]. DR–RNN is a physics-aware recurrent neural network for modeling the evolution of dynamical systems. The architecture of DR–RNN is inspired by iterative update techniques of line search methods where a fixed number of layers are stacked together to minimize the residual (or reduced residual) of the physical model under consideration. For subsurface flow models, we combine DR–RNN with proper orthogonal decomposition (POD) and discrete empirical interpolation method (DEIM) to reduce the computational complexity associated with high-fidelity numerical simulations and thus reduce the total cost of uncertainty quantification tasks. Our numerical evaluations show that DR–RNN combined with POD–DEIM provides an accurate and stable reduced models with a fixed computational budget that is much less than the computational cost of standard POD–Galerkin reduced model combined with DEIM.

References

[1] S. Chan, A. H. Elsheikh, A machine learning approach for efficient uncertainty quantification using multiscale methods, *Journal of Computational Physics*, 354, 2018, 493–511.

[2] J. N. Kani, A. H. Elsheikh, Reduced-Order Modeling of Subsurface Multi-phase Flow Models Using Deep Residual Recurrent Neural Networks, *Transport in Porous Media*, 126 (3), 2019, 713–741.

Machine learning approaches for the acceleration of the linear solver in PDE simulations

Markus Geveler, Hannes Ruelmann, and Stefan Turek

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While there is no doubt that Machine Learning empowers several scientific fields and industries and that it fires the hardware markets to adjust their portfolio to it, the major question asked when it comes to actually using it in Scientific (High Performance-) Computing is how to employ it alongside traditional methods *efficiently*. This imposes the necessity to not only adjust existing methods in the field of artificial neural networks to existing simulation pipelines but also for a careful performance modelling and -engineering. Both require a fundamental understanding of the design and theory of Machine Learning.

In the course of discretising Partial Differential Equations (PDEs) for real-world simulations at a certain point we have to deal with a high number of degrees of freedom leading to the global system matrix being large and sparse. Hence, iterative methods have to be chosen over direct ones. In the former everything breaks down to how clever the linear solver can adapt to the system to be solved and here using specially tailored solvers that are implemented in a target hardware-oriented way can be orders of magnitude faster than simple ones.

For this very general case of the solution of linear systems arising in simulations based on PDEs, we demonstrate simple and yet comprehensive Machine Learning methods [2], [1] that can accelerate these. For an early stage of development, we discuss their design, implementation, potential and efficiency in the context of modern compute hardware such as GPUs.

References

[1] RUELMANN, H., GEVELER, M., AND TUREK, S. On the prospects of using machine learning for the numerical simulation of PDEs: Training Neural Networks to assemble Approximate Inverses. *ECCOMAS newsletter issue 2018*, 27–32.

[2] RUELMANN, H. *Approximation von Matrixinversen mit Hilfe von Machine Learning*. Master's thesis, TU Dortmund, Dortmund, Germany, 2017.

On the use of machine learning in computational science and engineering

Jan S. Hesthaven

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During the last few years, the rapid development of machine learning techniques, eg advanced Gaussian process regression and neural networks, has led to remarkable advances in image classification, machine translation, and automatic game playing to name a few. However, for the simulation of complex problems in computational science and engineering, these advances are just beginning to have an impact and many challenges remain open.
In this presentation we discuss ways in which the remarkable power of such techniques in areas of regression and classification can be harvested to address problems that challenge traditional simulation techniques. Through a few concrete examples, ranging from image interpolation to intrusive but collaborative approaches, comprising a combination of classic simulations and machine learning, we show the potential for such emerging ideas in computational science and engineering and highlight challenges and open questions.
This work has been done in collaboration with D. Ray (EPFL, CH), Q. Chen (EPFL, CH), M. Guo (EPFL, CH), Z. Zhang (EPFL, CH), J. Magiers (Stuttgart, D), S. Ubbliani (USI, CH) and J. Yu (Beihang Uni, China).

Numerical precision in deep learning

Desmond Higham

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Modern deep learning computations are pushing the boundaries of large scale high performance computing. To deal with very high dimensional data sets, such as images and videos, and to train and implement hugely-parametrized models, the tools of deep learning must overcome severe hurdles. In particular, several studies have shown that a trained deep network for image classification can be fooled by carefully-chosen perturbations—a correctly categorized photo can be altered in a way that is imperceptible to the human eye but causes mystifying misclassification. In this talk we will focus on a closely-related issue concerning the sensitivity of deep network outputs: the extent to which results can be trusted if we account for floating-point rounding errors, especially when customized low-precision hardware is employed.

Constraint-aware neural networks for Riemann problems

Jim Magiera

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During the last few years many breakthroughs in the field of machine learning have been achieved. This has given rise to data driven modeling where the input–response relation of a complex/expensive model is learned with the help of machine learning algorithms to yield a reduced model [1, 2]. However, in many applications the learned/reduced model does not ensure physical constraints, like for example mass or momentum conservation.

Consequently, we want to develop a machine learning framework that respects physical constraints in the context of compressible flow governed by Euler equations. To this end, we investigate two methods to build neural networks that are constraint-aware, i.e. that they incorporate knowledge about underlying physical constraints during their generation. One of these methods satisfies the given constraints exactly, whereas the second method satisfies them only approximately.

To test these two methods, we consider three different model problems based on hyperbolic conservation law. For each of these model problems, the goal is to learn a network that acts as an Riemann solver in a numerical front-capturing scheme, while upholding the Rankine–Hugoniot conditions (e.g. mass, momentum and energy conservation across discontinuities). We compare the two constraint-aware methods with standard neural networks and test the performance of all methods applied to actual numerical simulations.

References

[1] F. Kissling and C. Rohde, *The Computation of Nonclassical Shock Waves in Porous Media with a Heterogeneous Multiscale Method: The Multidimensional Case*, Multiscale Modeling & Simulation, Vol. 13, Issue 4, 2015.

[2] J. Magiera and C. Rohde, *A Particle-Based Multiscale Solver for Compressible Liquid–Vapor Flow*, in: *Theory, Numerics and Applications of Hyperbolic Problems II* (ed. by C. Klingenberg and M. Westdickenberg), Springer International Publishing, 2018.

Scaling up deep learning for PDE-based models

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In numerous applications, forecasting relies on numerical solvers for partial differential equations (PDEs). Although the use of deep-learning techniques has been proposed, the uses have been restricted by the fact the training data are obtained using PDE solvers. Thereby, the uses were limited to domains, where the PDE solver was applicable, but no further. We present methods for training on small domains, while applying the trained models on larger domains, with consistency constraints ensuring the solutions are physically meaningful even at the boundary of the small domains. We demonstrate the results on an air-pollution forecasting model for Dublin, Ireland.
This is joint work with Philipp Haehnel (Harvard University), Julien Monteil (IBM Research), and Fearghal O'Donncha (IBM Research).

Some thoughts on neural networks, PDEs and data-driven discovery

Kaj Nyström

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In this talk I will discuss some experimental results/observations concerning unified neural network approximations to PDEs and how to augment methods for inverse problems for PDEs with neural networks. Time permitting I will also discuss data-driven discovery of PDEs.

Challenges and opportunities for numerical solvers of PDEs based on deep neural networks

Philipp Petersen

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Novel machine learning techniques based on deep learning have achieved remarkable results in many areas such as image classification and speech recognition. As a result, many scholars have started using them in areas which are not traditionally associated with machine learning. For instance, more and more researchers are employing deep neural networks to develop tools for the discretisation and solution of partial differential equations. Two reasons can be identified to be the driving forces behind the increased interest in neural networks in the area of the numerical analysis of PDEs. On the one hand, powerful approximation theoretical results have been established which demonstrate that neural networks can represent functions from the most relevant function classes with a minimal number of parameters. On the other hand, highly efficient machine learning techniques for the training of these networks are now available and can be used as a black box. In this talk, we will give an overview of some approaches towards the numerical treatment of PDEs with neural networks and study the two aspects above. We will recall classical and some novel approximation theoretical results and tie these results to PDE discretisation. Additionally, we will present theoretical results that show that neural networks can very efficiently solve parametric PDEs without curse of dimension if these parametric PDEs admit a sufficiently small reduced basis. Providing a counterpoint, we analyse the structure of network spaces and deduce considerable problems for the black box solver. In particular, we will identify a number of structural properties of the set of neural networks that render optimisation over this set especially challenging and sometimes impossible.

Rectified deep neural networks overcome the curse of dimensionality for nonsmooth value functions in zero-sum games of nonlinear stiff systems

Yufei Zhang

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In this talk, we establish that for a wide class of controlled stochastic differential equations (SDEs) with stiff coefficients, the value functions of corresponding zero-sum games can be represented by a DNN, whose complexity grows at most polynomially in both the dimension of the state equation and the reciprocal of the required accuracy. Such nonlinear stiff systems may arise, for example, from Galerkin approximations of controlled stochastic partial differential equations (SPDEs), or controlled PDEs with uncertain initial conditions and source terms. This implies that DNNs can break the curse of dimensionality in numerical approximations and optimal control of PDEs and SPDEs. The main ingredient of our proof is to construct a suitable discrete-time system to effectively approximate the evolution of the underlying stochastic dynamics. Similar ideas can also be applied to obtain expression rates of DNNs for value functions induced by stiff systems with regime switching coefficients and driven by general Lévy noise.
This is a joint work with Christoph Reisinger (Mathematical Institute, University of Oxford, United Kingdom).

References

[1] Christoph Reisinger and Yufei Zhang, *Rectified deep neural networks overcome the curse of dimensionality for nonsmooth value functions in zero-sum games of nonlinear stiff systems*, preprint, arXiv:1903.06652, 2019.

Panel discussion

Perspectives of machine learning algorithms in numerical analysis and scientific computing

Panelists:
Jan Hesthaven (EPFL, Switzerland)
Desmond Higham (University of Strathclyde, UK)

- What are the major mathematical challenges in this area?
- What areas of numerical analysis and scientific computing stand to benefit from machine learning/deep learning techniques?
- Can we identify some hot research themes/directions in this area?
- Are machine-learning algorithms and deep neural networks going to become 'universal solvers' that would replace our cherished FEM, BEM, etc.?
- Embed machine learning into numerical analysis or numerical analysis into machine learning?
- What computational resources are needed for
  (i) simple numerical experiments for model problems, and
  (ii) medium-range engineering applications?
- What existing (open-source) software can be useful?
- What educational resources are available for self-study (e.g., books, survey articles)?

In this panel discussion, we will address these and perhaps other relevant questions.

List of Participants

Muhammad Anwar	University of Nottingham	United Kingdom
Christoph Arthofer	University of Nottingham	United Kingdom
Matteo Bastiani	University of Nottingham	United Kingdom
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Adam Blakey	University of Nottingham	United Kingdom
Laura Bravo	University of Birmingham	United Kingdom
Keith Briggs	BT	England
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Kris van der Zee	University of Nottingham	United Kingdom
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Richard Widdowson	University of Nottingham	United Kingdom
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Lingyi Yang	University of Oxford	United Kingdom
Rawin Youngnoi	University of Birmingham	United Kingdom
Vitaly Zankin	Skolkovo Inst. of Sci. & Tech.	Russian Federation
Yufei Zhang	University of Oxford	United Kingdom