

PERSONAL INFORMATION

Davide Murari

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Gender Male | Date of birth 22 May 1996 | Nationality Italian

Personal Statement A PhD student in Numerical Analysis, mainly interested in the connections between neural networks, dynamical systems, and numerical analysis.

PHD THESIS

Candidate title: From dynamical systems to neural networks and back

Expected time of the defence: Middle of September 2024

Brief summary: The thesis investigates the connections between dynamical systems, neural networks, and numerical analysis techniques.

We first apply neural networks to discover the physics behind observed trajectories. We focus on Hamiltonian systems with holonomic constraints. To discover their dynamics while preserving the geometric structure of the problem, we rely on Lie group geometric numerical methods. This research further develops into analysing the problem of approximating the space-time evolution of partial differential equations with quadratic non-linear interaction terms, both from the experimental and theoretical points of view.

The second direction we pursue in the thesis is to interpret neural networks as discretisations of suitable differential equations to analyse them thanks to dynamical systems theory and with techniques typical of numerical analysis. We develop a framework to embed suitable desired properties into the neural network architecture. Two examples of such construction are forcing the network to have a controlled Lipschitz constant or preserving the sum of the input entries, i.e., conserving the mass of the input. This interpretation of neural networks also allows for a theoretical analysis of the expressivity power of some of them. We consider the case of networks based on composing maps which are discretisations of gradient flows and sphere-preserving dynamical systems, and show their theoretical universal approximation power. The experimental analysis of these structured networks primarily focuses on the Lipschitz constraint, which increases the robustness that networks have to adversarial perturbations. We develop robust neural networks based on gradient flow dynamics for image and graph node classification tasks.

The third line of research combines all these approaches to improve numerical methods for solving known differential equations. We propose symplectic neural networks for the solution of Hamiltonian ordinary differential equations to allow for the possibility of including data in the solution process. We then investigate how hybrid solution approaches based on classical numerical and data-driven methods could improve the numerical solver's efficiency for ODEs in the context of parallel-in-time integration.

PUBLICATIONS

- 2023 Celledoni, Elena, **Davide Murari**, Brynjulf Owren, Carola-Bibiane Schönlieb, and Ferdia Sherry. "Dynamical Systems–Based Neural Networks." *SIAM Journal on Scientific Computing* 45, no. 6 (2023): A3071-A3094.
- 2023 Celledoni, Elena, Andrea Leone, **Davide Murari**, and Brynjulf Owren. "Learning Hamiltonians of constrained mechanical systems." *Journal of Computational and Applied Mathematics* 417 (2023): 114608.
- 2021 Celledoni, Elena, Ergys Çokaj, Andrea Leone, **Davide Murari**, and Brynjulf Owren. "Dynamics of the N-fold Pendulum in the framework of Lie Group Integrators." In *European Consortium for Mathematics in Industry*, pp. 297-304. Cham: Springer International Publishing, 2021.
- 2021 Celledoni, Elena, Ergys Çokaj, Andrea Leone, **Davide Murari**, and Brynjulf Owren. "Lie group integrators for mechanical systems." *International Journal of Computer Mathematics* 99, no. 1 (2022): 58-88.

PREPRINTS

- 2023 Celledoni, Elena, Ergys Çokaj, Andrea Leone, Sigrid Leyendecker, **Davide Murari**, Brynjulf Owren, Rodrigo T. Sato Martín de Almagro, and Martina Stavole. "Neural networks for the approximation of Euler's elastica." (2023).
- 2023 Eliasof, Moshe, **Davide Murari**, Ferdia Sherry, and Carola-Bibiane Schönlieb. "Contractive Systems Improve Graph Neural Networks Against Adversarial Attacks." arXiv preprint arXiv:2311.06942 (2023).
- 2023 Sherry, Ferdia, Elena Celledoni, Matthias J. Ehrhardt, **Davide Murari**, Brynjulf Owren, and Carola-Bibiane Schönlieb. "Designing stable neural networks using convex analysis and ODEs." arXiv preprint arXiv:2306.17332 (2023).
- 2023 Celledoni, Elena, James Jackaman, **Davide Murari**, and Brynjulf Owren. "Predictions Based on Pixel Data: Insights from PDEs and Finite Differences." arXiv preprint arXiv:2305.00723 (2023).

NON-ARCHIVAL REPORTS

- 2022 **Murari, Davide**, Elena Celledoni, Brynjulf Owren, Ferdia Sherry, and Carola-Bibiane Schönlieb. "Structure preserving neural networks based on ODEs." *NeurIPS 2022 Workshop DLDE*, 2022.

EDUCATION

- 2020-Current date **PhD in Numerical Analysis**, Norwegian University of Science and Technology, with a focus on the interconnections between dynamical systems, geometric numerical integration of ODEs and neural networks
- 2018-2020 **Master in Mathematics** (L-40), University of Studies of Verona, Italy. Graduated in July 2020, with a thesis on integrability of non-Hamiltonian vector fields titled "Integrable non-Hamiltonian systems: from B-integrability to Euler-Jacobi Theorem and back".
- September 2019 - January 2020 **Erasmus+**, University of Côté D'Azur, Nice, focused mostly on numerical and functional analysis courses.

July 2019 Attendance of an **ECMI Modelling Week**, which took place at Grenoble (FR). The goal of the project was to analyse if the floor of a room satisfies some German evenness standard starting from measured data.

2015-2018 **Bachelor in Applied Mathematics** (L-35), University of Studies of Verona, Italy. Graduated with a thesis on dynamical billiards, with the title translating to "An overview of ergodic theory and dynamical billiards".

PEER REVIEW

Reviewer for the following scientific Journals:

- Calcolo
- IMA Journal of Applied Mathematics
- IMA Journal of Numerical Analysis

ORGANISED MINI-SYMPOSIA

Collaborated on the organisation of two mini-symposia:

- Currently organising a mini-symposium at the conference SciCADE 2024, July 15 2024 - July 19 2024. The organisation group is composed of Elena Celledoni, James Jackaman, Brynjulf Owren, Carola Schönlieb, Ferdia Sherry and me. The title of the mini-symposium is "Dynamical systems, structure preservation and deep learning".
- Mini-symposium at the conference "Geometric Science of Information", St. Malo, France, August 30 2023 - September 1 2023. The organisation group was composed of Elena Celledoni, James Jackaman, Brynjulf Owren, and me. The title of the mini-symposium is "Deep Learning: Methods, Analysis and Applications to Mechanical systems".

EDITORIAL WORK

2021-2022 Guest editor for the ECMI Annual reports of the years 2021 and 2022.

TEACHING EXPERIENCE

Fall 2023 Teaching assistant in the course "Numerical Solution of Partial Differential Equations Using Element Methods - TMA4220" at NTNU.

March 2023 Grading of 100 exams in the course "Mathematical methods 3 - IMAT2100" at NTNU.

December 2022 Grading of 200 exams in the course "Matematics 4N - TMA4130" at NTNU.

Fall 2022 Teaching assistant in the course "Numerical Solution of Partial Differential Equations Using Element Methods - TMA4220" at NTNU.

Spring 2022 Teaching assistant in the course "Optimization 1 - TMA4180" at NTNU.

Fall 2021 Teaching assistant in the course "Numerical Solution of Partial Differential Equations Using Element Methods - TMA4220" at NTNU.

- Spring 2021 Teaching assistant in the course "Differential Equations and Dynamical Systems - TMA4165" at NTNU.
- December 2020 Grading of 100 exams in the course "Programming and Numerics - TDT4127" at NTNU.
- Spring 2020 Student assistant in the course "Dynamical systems" at the University of Verona.

TALKS AND ATTENDED EVENTS

- December 2023 (Invited talk) Final Workshop of RIBA Project 2019, University of Verona, Italy. Talk titled "Contractive Systems Inspired GNNs".
- September 2023 (Invited talk at a mini-symposium) TES Conference on Mathematical Optimization for Machine Learning, Berlin, Germany. Talk titled "Predictions Based on Pixel Data".
- August 2023 (Invited talk at a mini-symposium) ICIAM 2023, Tokyo, Japan (Online talk). Talk titled "Structured neural networks and some applications".
- June 2023 (Invited talk at a mini-symposium) ECMI Conference 2023, Wroklav, Poland. Talk titled "Learning Hamiltonians of constrained mechanical systems".
- June 2023 (Invited talk at a mini-symposium) FoCM 2023, Paris, France. Talk titled "Structured neural networks and some applications to dynamical systems".
- May 2023 The mathematical and statistical foundation of future data-driven engineering, Newton-Institute, Cambridge, England. Talk titled "A numerical analysis perspective on neural networks".
- March 2023 (Group seminar) Cambridge Image Analysis Seminar, Cambridge, England. Talk titled "From neural networks to dynamical systems and back".
- March - May 2023 (Thematic semester) "The mathematical and statistical foundation of future data-driven engineering" Newton-Institute, Cambridge, England.
- February 2023 (Invited talk at a mini-symposium) SIAM CSE, Amsterdam, Netherlands. Talk titled "Structured neural networks and their relevance for mechanical systems".
- December 2022 (Invited talk) Theoretical and Computational aspects of Dynamical Systems (HB60), Trysil, Norway. Talk titled "Dynamical systems' based neural networks".
- July 2022 (Invited talk) SciCADE, Reykjavík, Iceland. Talk titled "Structure preserving neural networks coming from ODE models".
- July 2022 (Invited talk) Young Researchers Seminars, Maths Applications & Models, Verona, Italy. Talk titled "Learning Hamiltonians of constrained mechanical systems".
- June 2022 (Internal talk) DNA Seminar, Trondheim, Norway. Talk titled "Neural networks modelled by dynamical systems".
- May 2022 (Invited talk) Machine Learning and Dynamical Systems Seminar, Online. Talk titled "Learning Hamiltonians of constrained mechanical systems".
- April 2022 (Invited talk) Veronesi Tutti Math Seminar, Online. Talk titled "Some connections between dynamical systems and neural networks".

- March 2022 Manifolds and Geometric Integration Colloquium 2022, Ilsetra, Norway. Talk titled "Robustness of neural networks for classification problems".
- November 2021 (Workshop) Computational Mathematics and Machine Learning Workshop, Leiden, Netherlands. Talk titled "Learning the Hamiltonian of some constrained mechanical systems"
- October 2021 (Thematic semester) Mathematics of deep learning, at the Newton Institute, Cambridge, UK.
- September 2021 (Invited talk at a mini-symposium) NUMDIFF-16, Halle, Germany. Talk titled "Learning the Hamiltonian of some classes of mechanical systems"
- February 2021 Manifolds and Geometric Integration Colloquium 2021, Ilsetra, Norway. Talk titled "Lie group integrator's approach to the N-fold pendulum".

PRESENTED POSTERS

- January 2024 Geilo Winter School, Geilo, Norway. Poster titled "Contractive Systems Improve Graph Neural Networks Against Adversarial Attacks".
- December 2022 The Symbiosis of Deep Learning and Differential Equations (DLDE) - II, NeurIPS Workshop. Poster titled "Structure preserving neural networks based on ODEs".

LANGUAGE SKILLS

- Mother tongue Italian
- Other languages
- English Fluent (B2)
- Norwegian (Bokmål) Intermediate (B1)

COMMUNICATION SKILLS

Interested in communicating mathematics, sharing content about various topics in this field with a project in Italian language:

- in written format on the blog: <https://www.mathone.it/>,
- in video format on the YouTube channel: <https://www.youtube.com/@MathoneVideo>.