Professor Pietro Liò

Position	I am Full Professor of Computational Biology in the Artificial Intelligence Division of the Department of Computer Science and Technology of the University of Cambridge
Personal	citizenship: Italian; Married, one daughter
Document	Curriculum past 4 years achievements: 2019-2023

Affiliations

Department of Computer Science and Technology (Cambridge), J. Thomson Avenue, CB03FD Cambridge
email
tel

Other Affiliations

Cambridge Center for AI and Medicine (Cambridge)
Fellow and member of the Council of Clare Hall College (Cambridge).

Research Interests

Research Interests	AI methodology, AI and Medicine, Bioinformatics and Computational Biology
Which AI methodology I focus on	Graph representation learning and higher order graphs; neurosymbolic; explainability; diffusion models

Which targets for AI and medicine I focus on	Develop methodology in Artificial Intelligence and computational Biology that can lead to useful applications and be respectful of societal values particularly cancer and neurodegenerative diseases; developing methods for the integration of multi scale heterogeneous data; model the overall progression of complex diseases which is critical to the timing of therapeutic interventions and design of effective clinical trials; incorporation of models of uncertainties and counterfactuals and go beyond the hypothesis confirmation towards the generation of new hypotheses; develop a fully trustworthy AI, to assist, help doctor and patients
Which targets of Bioinformatics and Computational Biology I focus on	Biological Complexity; Theoretic Information in Biology; Evo-Devo; single cell; dynamical biosystems; Computational Biology as the new AI

Past Positions

Lecturer (part time Lecturer), Chemistry Dept, University Firenze; course held in years: 1988,89,90; fellowship Institute of National Physics of Matter INFM (1995); Research Associate in Statistical Epidemiology, Princess Anne Hospital, University of Southampton. (1996-1997); Research Associate, Dept. of Genetics, Cambridge; (1998-2000); Research Associate Univ. Cambridge Dept. of Zoology, Cambridge, 2001; Research associate at the European Bioinformatics Institute (2002); Lecturer in Bioinformatics algorithms at the Computer Laboratory, University of Cambridge and affiliated Faculty member of the Centre for Computational Biology, Department of Mathematics, University of Cambridge (2004), Director of studies of Computer Science of Fitzwilliam College (2004-2014); Senior Lecturer, The Computer Laboratory, University of Cambridge (2007); Reader in Computational medicine at the Computer Laboratory, University of Cambridge (2013); - Full Professor in Computational Biology (2018).

Visiting Positions ($>$ 1 month)

University of Padova, University of Toronto and Fields Institute (Canada), University of UCSC (USA), University of Texas (College Station, USA).

International Activities

2024	Member of Panel for Activities of Pasteur Institutes (France)
2022	Member of Panel for Activities of Adapta (Science Foundation Ireland)
2021	Member of Panel for Italian ERC Awards (CNR, Italy)

Awards - Honours (recent)

2022	Fellow of the Asia-Pacific Artificial Intelligence Association (AAIA)
2021	Fellow of the Academia Europaea
2019	Member of Ellis, the European Lab for Learning & Intelligent Systems
2023	Listed in the “A standardized citation metrics author database annotated for scientific field” (doi.org/10.1371/journal.pbio.3000384)

	Listed in the top Italian Scientists: `www.topitalianscientists.org/TIS_HTML/Top_Italian_Scientists_Computer_Sciences.htm`
Erdos n 3	www.csauthors.net/distance/pietro-lio/paul-erdos

Invited Talks

23 April 2024	Invited talk, Department of Computer Science, Bocconi University, Milano
15 April 2024	Turing Lecture, Invited talk, Turing-AI, Queen's University, Belfast
9 April 2024	Invited talk, Department of Computer Science, University of Padova
22 March 2024	Invited talk, AI4H conference, Padova
8 September2023	Invited talk, school of BioPhotonics and AI, Firenze
August 2023	lecture at the IoT & AI for Sustainable Global Health and Wellbeing 2023 summer school, Cambridge
06-07 July	Invited, 6th Machine Learning and AI in Bio(Chemical) Engineering Conference
21 June	Invited, Deep Learning 2023, Trento, Italy
7th June	Invited talk, 2023 IEEE World AI IoT Congress (AIIoT) (online)
June7-10	Teaching First Doctoral Summer School in Data Science, Accounting & Management Summer school, Paestum, Italy
June 6	Invited talk, WIRN2023, Vietri, Italy
June 3, 2023	Keynote talk, IEEE AIIoT 2023
May 2023	Invited talk, IEEE MetroLivEnv
March 2023	Invited talk - Pujiang Innovation Forum (Online)
March 2023	Turing Lecture, Invited talk AI- Turing Institute, Teesside
March 2023	Invited talk - Physics of Life, Harrogate
6 March 2023	Invited talk - Statistical learning on LARge scale GRaphs (LARGR), Inria, Universite de Lille
December 2022	Invited Talk, Istituto Italiano di Cultura Italiano, ENCOUNTERS: across sciences and humanities
Sept 2022	Invited talk at the Summer School on AI and Medicine, Cambridge (online)
Sept 2022	Invited talk at the School of Biophotonics, Florence, Italy
28 June 2022	Invited talk - ShanghaiTech SIST Distinguished Lecture, at the Jiao Tong University, Shanghai, China
Jun 2022	Invited talk at CMBE21 (7th International Conference on Computational and Mathematical Biomedical Engineering); Politecnico di Milano
Dec 2021	Invited talk at Int. Workshop on Future Computing and Networks, Changchun, China
Jan 2021	Invited talk: Next Generation Internet, NGI.eu, Forward workshop: The Future of search: Search and (hyper) locality, Search in/and Internet of Things, Search and Ethics - European Community

Jan 2020 Invited talk at the 21st International Conference on Distributed Computing and Networking, ICDCN Conference, Kolkata

Sept 2019 Invited talk on AI and data social awareness, MyData2019, Helsinki

Research: Active Grants

-2023 Wisdom, WELL-BEING IMPROVEMENT THROUGH THE INTEGRATION OF HEALTHCARE AND RESEARCH DATA AND MODELS WITHOUT BORDER FOR CHRONIC IMMUNE-MEDIATED DISEASES, Horizon Europe, Trophy (G112412 NRAG/752), Horizon Europe UKRI Underwrite Innovate, Title: Ultrafast Holographic FTIR Microscopy (2022-2026); £ 294k; Charm (G113952 NRAG/750), Horizon Europe UKRI Underwrite Innovate (2022-2026), title: Chemometric Histopathology via Coherent Raman Imaging for Precision Medicine, £ 275k; GO-DS21, European Commission Horizon 2020 (H2020) Societal Challenges, Go-Ds21 : Gene Overdosage And Comorbidities During The Early Lifetime In Down Syndrome (2020-2024), £400k; Few PhD fellowships sponsored by Astrazeneca (2 students; 1 through CCAIM), GSK (2 students; 1 through CCAIM); CMIH: Cambridge Mathematics Of Information In Healthcare (Cmih), EPSRC, 2020-2023

Governance Activities

2024 Member of the Student Complaints and Appeal Committee of the University of Cambridge; member of the Postdoc mentorship scheme of the University of Cambridge

2021-2023 Member of the Faculty Board of the Dept of Computer Science and Technology; University of Cambridge Steering committee Big Data (The Cambridge Centre for Data-Driven Discovery (C2D3)); University of Cambridge - High performance computing panel; University of Cambridge Computational Biology Steering Committee; Member of the Student Complaints and Appeal Committee of the University of Cambridge; member of the panel for professorships at the Dept of Computer Science and Technology, University of Cambridge; examiner of ACS MPhil, Dept of Computer Science and Technology, University of Cambridge; Member of School of Technology STEC PhD Fellowship Calls Team

Service to the academic community outside the University

-2023 Member of panel for professorship on Machine Learning and Biology, Copenhagen, Denmark (September 2022); External Examiner at the University of Newcastle for the MSc Bioinformatics, MSc Computational Neuroscience and Neuroinformatics, MSc Computational Systems Biology (2017-2021); Member of the committee of the VPHiUK.Organiser and co-organizer of scientific conferences and workshops: 08/12/2022 Learning on Graph (LoG) Cambridge.

Service to the Underpriviledge schools

-2023 Teaching Sutton College Summer School, Cambridge

-2022 Teaching Sutton College Cambridge

Collaborations with Industry

2022	member AI panel of GSK

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Teaching and supervision

-2023	ACS MPhil course on Graph Representation Networks; Bioinformatics Algorithms -Undergraduate -Dept Computer science and technology
-2024	38 PhD students have been awarded the PhD, >40 MPhil students supervised (MPhil in advanced computing; Part III Systems biology; MPhil in computational Biology; Part III Physics); >20 PartII students

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Dissemination to the broader public (only recent)

2022-2024	Organisation of CS AI SIG - Special Interest Group, 1/term at Clare Hall College, Cambridge
Nov 2020	Lecture on AI and medicine, FuturoRemoto exhibition, Napoli
Oct 2020	Talk on AI and medicine, TEDxCambridge University
Jul 2019	Bioinformatics for Kids, CambridgeSpark - Cambridge

Publications from Cambridge University Symplectic database

orcid	0000-0001-8956-9815
Erdős number	3
–2024	>600 publications in journals and international conferences; arxiv and bioarxiv as preliminary deposit; H-index = 71 (Google Scholar); i10-index=371; >54000 citations. `https://scholar.google.co.uk/citations?user=3YrWf7EAAAAJ&hl=en&oi=ao`; `https://orcid.org/0000-0002-0540-5053`; `noteanotherOrcidunderforenamewithdifferentaccent`

Publications

[1] F Ceccarelli, SB Holden, and P Liò. Mugi-mri: Enhancing breast cancer classification through multiplex graph neural networks in dce-mri. Yokohama, Japan.

[2] M Li, A Micheli, YG Wang, S Pan, P Lió, GS Gnecco, and M Sanguineti. Guest editorial: Deep neural networks for graphs: Theory, models, algorithms, and applications. *IEEE Trans. Neural Networks Learn. Syst.*, 35(4):4367–4372, Apr 2024.

[3] F Bardozzo, A Terlizzi, C Simoncini, P Lió, and R Tagliaferri. Elegans-ai: How the connectome of a living organism could model artificial neural networks. *Neurocomputing*, 584, Jun 2024.

[4] T Dong, M Jamnik, and P Liò. Sphere neural-networks for rational reasoning, Mar 2024.

[5] S Somathilaka, A Ratwatte, S Balasubramaniam, MC Vuran, W Srisa-an, and P Liò. Wet tinyml: Chemical neural network using gene regulation and cell plasticity, Mar 2024. Accepted as a full paper by the tinyML Research Symposium 2024.

[6] K Huang, W Cao, H Ta, X Xiao, and P Liò. Optimizing polynomial graph filters: A novel adaptive krylov subspace approach, Mar 2024.

[7] A Defilippo, P Veltri, P Lio', and PH Guzzi. Leveraging graph neural networks for supporting automatic triage of patients, Mar 2024.

[8] E Lawrence, A El-Shazly, S Seal, CK Joshi, P Liò, S Singh, A Bender, P Sormanni, and M Greenig. Understanding biology in the age of artificial intelligence, Mar 2024.

[9] D Buterez, JP Janet, SJ Kiddle, D Oglic, and P Lió. Transfer learning with graph neural networks for improved molecular property prediction in the multi-fidelity setting. *Nat Commun*, 15(1):1517, Feb 2024.

[10] D Buterez, JP Janet, SJ Kiddle, D Oglic, and P Lió. Transfer learning with graph neural networks for improved molecular property prediction in the multi-fidelity setting. *Nature Communications*, 15(1).

[11] F Ceccarelli, L Giusti, S Holden, and P Lio. Integrating structure and sequence: Protein graph embeddings via gnns and llms. Feb 2024.

[12] X Zhao, Z Li, M Shen, G-B Stan, P Liò, and Y Zhao. Enhancing real-world complex network representations with hyperedge augmentation, Feb 2024. Preprint. Under review. 17 pages, 4 figures, 14 tables. arXiv admin note: text overlap with arXiv:2306.05108.

[13] D Buterez, JP Janet, D Oglic, and P Lio. Masked attention is all you need for graphs, Feb 2024.

[14] T Papamarkou, T Birdal, M Bronstein, G Carlsson, J Curry, Y Gao, M Hajij, R Kwitt, P Liò, PD Lorenzo, V Maroulas, N Miolane, F Nasrin, KN Ramamurthy, B Rieck, S Scardapane, MT Schaub, P Veličković, B Wang, Y Wang, G-W Wei, and G Zamzmi. Position paper: Challenges and opportunities in topological deep learning, Feb 2024.

[15] N Mumenin, MA Yousuf, MA Nashiry, AKM Azad, SA Alyami, P Lio', and MA Moni. Asdnet: A robust involution-based architecture for diagnosis of autism spectrum disorder utilising eye-tracking technology. *IET Computer Vision*, Jan 2024.

[16] A Bazaga, P Liò, and G Micklem. Hyperbert: Mixing hypergraph-aware layers with language models for node classification on text-attributed hypergraphs, Feb 2024. 11 pages, 2 figures.

[17] D Georgiev, P Liò, and D Buffelli. The deep equilibrium algorithmic reasoner, Feb 2024.

[18] K Didi, F Vargas, SV Mathis, V Dutordoir, E Mathieu, UJ Komorowska, and P Lio. A framework for conditional diffusion modelling with applications in motif scaffolding for protein design, Dec 2023. 9 pages.

[19] A Duval, SV Mathis, CK Joshi, V Schmidt, S Miret, FD Malliaros, T Cohen, P Liò, Y Bengio, and M Bronstein. A hitchhiker's guide to geometric gnns for 3d atomic systems, Dec 2023.

[20] A Bazaga, P Liò, and G Micklem. Language model knowledge distillation for efficient question answering in spanish, Dec 2023. ICLR 2024 Tiny Paper (6 pages, 2 tables).

[21] G Bernárdez, L Telyatnikov, E Alarcón, A Cabellos-Aparicio, P Barlet-Ros, and P Liò. Topological network traffic compression. In *GNNet 2023 - Proceedings of the 2nd Graph Neural Networking Workshop 2023*, pages 7–12, Dec 2023.

[22] AFD Villaforesta, LC Magister, P Barbiero, and P Liò. Digital histopathology with graph neural networks: Concepts and explanations for clinicians, Dec 2023.

[23] J Yang and P Liò. Unsupervised adaptive implicit neural representation learning for scan-specific mri reconstruction, Dec 2023.

[24] J Yang and P Liò. Dual-domain multi-contrast mri reconstruction with synthesis-based fusion network, Dec 2023.

[25] L Liu, Y Cheng, Z Deng, S Wang, D Chen, X Hu, P Liò, C-B Schönlieb, and A Aviles-Rivero. Trafficmot: A challenging dataset for multi-object tracking in complex traffic scenarios, Nov 2023. 17 pages, 7 figures.

[26] K Huang and P Liò. An effective universal polynomial basis for spectral graph neural networks, Nov 2023.

[27] D Buterez, JP Janet, SJ Kiddle, D Oglic, and P Liò. Modelling local and general quantum mechanical properties with attention-based pooling. *Commun Chem*, 6(1):262, Nov 2023.

[28] A Marinoni, P Lio', A Barp, C Jutten, and M Girolami. Improving embedding of graphs with missing data by soft manifolds, Nov 2023.

[29] I Brant, A Norcliffe, and P Liò. Fourier neural differential equations for learning quantum field theories, Nov 2023. 9 pages, 6 figures.

[30] X Bi, S Tang, Z Yang, X Deng, B Xiao, and P Lio. Mmctnet: Multi-modal cony-transformer network for predicting good and poor outcomes in cardiac arrest patients. In *Computing in Cardiology*, Jan 2023.

[31] J Jürß, LC Magister, P Barbiero, P Liò, and N Simidjievski. Everybody needs a little help: Explaining graphs via hierarchical concepts, Nov 2023. 33 pages, 16 figures, accepted at the NeurIPS 2023 GLFrontiers Workshop.

[32] Z Shen, Y Cheng, RH Chan, P Liò, C-B Schönlieb, and AI Aviles-Rivero. Trident: The nonlinear trilogy for implicit neural representations, Nov 2023.

[33] M Zhu, S Stanivuk, A Petrovic, M Nikolic, and P Lio. Incorporating llm priors into tabular learners, Nov 2023. Table Representation Learning Workshop at NeurIPS 2023.

[34] Y Lu, HSDO Borde, and P Liò. Ames: A differentiable embedding space selection framework for latent graph inference, Nov 2023.

[35] S Kidwai, P Barbiero, I Meijerman, A Tonda, P Perez-Pardo, P Lio, AH van der Maitland-Zee, DL Oberski, AD Kraneveld, and A Lopez-Rincon. A robust mrna signature obtained via recursive ensemble feature selection predicts the responsiveness of omalizumab in moderate-to-severe asthma. *Clin Transl Allergy*, 13(11):e12306, Nov 2023.

[36] L Liu, Y Cheng, D Chen, J He, P Liò, C-B Schönlieb, and AI Aviles-Rivero. Traffic video object detection using motion prior, Nov 2023. 11 pages, 4 figures.

[37] M Zhu, K Kobalczyk, A Petrovic, M Nikolic, MVD Schaar, B Delibasic, and P Lio. Tabular few-shot generalization across heterogeneous feature spaces, Nov 2023. Tabular learning, Deep learning, Few shot learning.

[38] D Crisostomi, I Cannistraci, L Moschella, P Barbiero, M Ciccone, P Liò, and E Rodolà. From charts to atlas: Merging latent spaces into one, Nov 2023. To appear in the NeurReps workshop @ NeurIPS 2023.

[39] SI Nayan, MH Rahman, MM Hasan, SMRH Raj, MAA Almoyad, P Liò, and MA Moni. Network based approach to identify interactions between type 2 diabetes and cancer comorbidities. *Life Sci*, 335:122244, Dec 2023.

[40] J Chen, Y Wang, C Bodnar, R Ying, P Lio, and YG Wang. Dirichlet energy enhancement of graph neural networks by framelet augmentation, Nov 2023.

[41] Y Jiang, Q Ding, YG Wang, P Liò, and X Zhang. Vision graph u-net: Geometric learning enhanced encoder for medical image segmentation and restoration. *Inverse Problems and Imaging*, 2023, Nov 2023.

[42] A Bazaga, P Liò, and G Micklem. Sqlformer: Deep auto-regressive query graph generation for text-to-sql translation, Oct 2023. 11 pages, 4 figures.

[43] L Telyatnikov, MS Bucarelli, G Bernardez, O Zaghen, S Scardapane, and P Lio. Hypergraph neural networks through the lens of message passing: A common perspective to homophily and architecture design, Oct 2023.

[44] JD Boom, M Greenig, P Sormanni, and P Liò. Score-based generative models for designing binding peptide backbones, Oct 2023.

[45] I Duta, G Cassarà, F Silvestri, and P Liò. Sheaf hypergraph networks, Sep 2023. Accepted at Neural Information Processing Systems (NeurIPS 2023).

[46] A Bazaga, P Liò, and G Micklem. Unsupervised pretraining for fact verification by language model distillation, Sep 2023. ICLR 2024 Camera Ready.

[47] X Lu, C Liu, S Zhu, Y Mao, P Lio, and P Hui. Rlpto: A reinforcement learning-based performance-time optimized task and resource scheduling mechanism for distributed machine learning. *IEEE Transactions on Parallel and Distributed Systems*, 34(12):3266–3279, Dec 2023.

[48] T Shadbahr, M Roberts, J Stanczuk, J Gilbey, P Teare, S Dittmer, M Thorpe, RV Torné, E Sala, P Lió, M Patel, J Preller, AIX-COVNET Collaboration, JHF Rudd, T Mirtti, AS Rannikko, JAD Aston, J Tang, and C-B Schönlieb. The impact of imputation quality on machine learning classifiers for datasets with missing values. *Commun Med (Lond)*, 3(1):139, Oct 2023.

[49] COVID-19 Host Genetics Initiative. A second update on mapping the human genetic architecture of covid-19. *Nature*, 621(7977):E7–E26, Sep 2023.

[50] M Mamalakis, HD Vareilles, A Al-Manea, SC Mitchell, I Arartz, LE Morch-Johnsen, J Garrison, J Simons, P Lio, J Suckling, and G Murray. An explainable three dimension framework to uncover learning patterns: A unified look in variable sulci recognition, Sep 2023.

[51] AA Chowdhury, SM Hasan Mahmud, KK Shahjalal Hoque, K Ahmed, FM Bui, P Lio, MA Moni, and FA Al-Zahrani. Stackfbas: Detection of fetal brain abnormalities using cnn with stacking strategy from mri images. *Journal of King Saud University - Computer and Information Sciences*, 35(8), Sep 2023.

[52] X Zou, X Zhao, P Liò, and Y Zhao. Will more expressive graph neural networks do better on generative tasks?, Aug 2023. 2nd Learning on Graphs Conference (LoG 2023). 26 pages, 5 figures, 11 tables.

[53] R Bergna, F Opolka, P Liò, and JM Hernandez-Lobato. Graph neural stochastic differential equations, Aug 2023. 9 main pages, 6 of appendix (15 in total), submitted for the Learning on Graph (LoG) conference.

[54] N Faruqui, MA Yousuf, M Whaiduzzaman, AKM Azad, SA Alyami, P Liò, MA Kabir, and MA Moni. Safetymed: A novel iomt intrusion detection system using cnn-lstm hybridization. *Electronics (Switzerland)*, 12(17), Sep 2023.

[55] J Torge, C Harris, SV Mathis, and P Lio. Diffhopp: A graph diffusion model for novel drug design via scaffold hopping, Aug 2023.

[56] C Harris, K Didi, AR Jamasb, CK Joshi, SV Mathis, P Lio, and T Blundell. Benchmarking generated poses: How rational is structure-based drug design with generative models?, Aug 2023.

[57] E De Maria, J Despeyroux, A Felty, P Liò, C Olarte, and A Bahrami. Computational logic for biomedicine and neurosciences. In *Symbolic Approaches to Modeling and Analysis of Biological Systems*, pages 187–234. Aug 2023.

[58] G Ciravegna, F Giannini, P Barbiero, M Gori, P Lio, M Maggini, and S Melacci. Learning logic explanations by neural networks. In *Compendium of Neurosymbolic Artificial Intelligence*, pages 547–558. Aug 2023.

[59] Z Wang, Q Gao, X Yi, X Zhang, Y Zhang, D Zhang, P Liò, C Bain, R Bassed, S Li, Y Guo, S Imoto, J Yao, RJ Daly, and J Song. Surformer: An interpretable pattern-perceptive survival transformer for cancer survival prediction from histopathology whole slide images. *Comput Methods Programs Biomed*, 241:107733, Nov 2023.

[60] G Ciravegna, F Giannini, P Barbiero, M Gori, P Lio, M Maggini, and S Melacci. Chapter 25. learning logic explanations by neural networks. In *Frontiers in Artificial Intelligence and Applications*. IOS Press, Jul 2023.

[61] T Azevedo, RAI Bethlehem, DJ Whiteside, N Swaddiwudhipong, JB Rowe, P Lió, T Rittman, and Alzheimer's Disease Neuroimaging Initiative. Identifying healthy individuals with alzheimer's disease neuroimaging phenotypes in the uk biobank. *Commun Med (Lond)*, 3(1):100, Jul 2023.

[62] R Jain, P Veličković, and P Liò. Neural priority queues for graph neural networks, Jul 2023.

[63] R Viñas, CK Joshi, D Georgiev, P Lin, B Dumitrascu, ER Gamazon, and P Liò. Hypergraph factorization for multi-tissue gene expression imputation. *Nat Mach Intell*, 5(7):739–753, Jul 2023.

[64] X Zhang, L Wang, J Helwig, Y Luo, C Fu, Y Xie, M Liu, Y Lin, Z Xu, K Yan, K Adams, M Weiler, X Li, T Fu, Y Wang, H Yu, Y Xie, X Fu, A Strasser, S Xu, Y Liu, Y Du, A Saxton, H Ling, H Lawrence, H Stärk, S Gui, C Edwards, N Gao, A Ladera, T Wu, EF Hofgard, AM Tehrani, R Wang, A Daigavane, M Bohde, J Kurtin, Q Huang, T Phung, M Xu, CK Joshi, SV Mathis, K Azizzadenesheli, A Fang, A Aspuru-Guzik, E Bekkers, M Bronstein, M Zitnik, A Anandkumar, S Ermon, P Liò, R Yu, S Günnemann, J Leskovec, H Ji, J Sun, R Barzilay, T Jaakkola, CW Coley, X Qian, X Qian, T Smidt, and S Ji. Artificial intelligence for science in quantum, atomistic, and continuum systems, Jul 2023.

[65] G Dominici, P Barbiero, LC Magister, P Liò, and N Simidjievski. Sharcs: Shared concept space for explainable multimodal learning, Jul 2023.

[66] Y Lishkova, P Scherer, S Ridderbusch, M Jamnik, P Liò, S Ober-Blöbaum, and C Offen. Discrete lagrangian neural networks with automatic symmetry discovery. *IFAC-PapersOnLine*, 56(2):3203–3210, Jul 2023.

[67] K Yi, B Zhou, Y Shen, P Liò, and YG Wang. Graph denoising diffusion for inverse protein folding, Jun 2023. NeurIPS 2023.

[68] A Margeloiu, N Simidjievski, P Liò, and M Jamnik. Weight predictor network with feature selection for small sample tabular biomedical data. In *Proceedings of the 37th AAAI Conference on Artificial Intelligence, AAAI 2023*, volume 37, pages 9081–9089, Jun 2023.

[69] A Margeloiu, N Simidjievski, P Liò, and M Jamnik. Weight predictor network with feature selection for small sample tabular biomedical data. *Proceedings of the AAAI Conference on Artificial Intelligence*, 37(8):9081–9089.

[70] H Xuanyuan, P Barbiero, D Georgiev, LC Magister, and P Liò. Global concept-based interpretability for graph neural networks via neuron analysis. *Proceedings of the 37th AAAI Conference on Artificial Intelligence, AAAI 2023*, 37:10675–10683, Jun 2023.

[71] F Bardozzo, A Terlizzi, P Lio, and R Tagliaferri. Elegansai: how a biological neural network would compare with artificial networks?, Jun 2023.

[72] A Bisercic, M Nikolic, MVD Schaar, B Delibasic, P Lio, and A Petrovic. Interpretable medical diagnostics with structured data extraction by large language models, Jun 2023.

[73] Z Li, X Zhao, M Shen, G-B Stan, P Liò, and Y Zhao. Hybrid graph: A unified graph representation with datasets and benchmarks for complex graphs, Jun 2023. 16 pages, 5 figures, 11 tables.

[74] F Ceccarelli, L Giusti, SB Holden, and P Liò. Neural embeddings for protein graphs, Jun 2023. 10 pages, 5 figures.

[75] FL Opolka, Y-C Zhi, P Liò, and X Dong. Graph classification gaussian processes via spectral features, Jun 2023.

[76] L Giusti, T Reu, F Ceccarelli, C Bodnar, and P Liò. Cin++: Enhancing topological message passing, Jun 2023. 21 pages, 9 figures.

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[78] A Breger, I Selby, M Roberts, J Babar, E Gkrania-Klotsas, J Preller, L Escudero Sánchez, AIX-COVNET Collaboration, JHF Rudd, JAD Aston, JR Weir-McCall, E Sala, and C-B Schönlieb. A pipeline to further enhance quality, integrity and reusability of the nccid clinical data. *Sci Data*, 10(1):493, Jul 2023.

[79] X Mei, Y Yang, M Li, C Huang, K Zhang, and P Lió. A feature reuse framework with texture-adaptive aggregation for reference-based super-resolution, Jun 2023.

[80] F Caso, G Trappolini, A Bacciu, P Liò, and F Silvestri. Renormalized graph neural networks, Jun 2023.

[81] K Bujel, Y Gideoni, CK Joshi, and P Liò. Group invariant global pooling, May 2023.

[82] CK Joshi, AR Jamasb, R Viñas, C Harris, S Mathis, A Morehead, and P Liò. grnade: Geometric deep learning for 3d rna inverse design, May 2023. Previously titled 'Multi-State RNA Design with Geometric Multi-Graph Neural Networks', presented at ICML 2023 Computational Biology Workshop.

[83] R Viñas, P Scherer, N Simidjievski, M Jamnik, and P Liò. Spatio-relational inductive biases in spatial cell-type deconvolution, 2023.

[84] D Georgiev, D Numeroso, D Bacciu, and P Liò. Neural algorithmic reasoning for combinatorial optimisation, May 2023.

[85] F Giannini, S Fioravanti, O Keskin, AM Lupidi, LC Magister, P Lio, and P Barbiero. Interpretable graph networks formulate universal algebra conjectures, May 2023.

[86] G Wölflein, LC Magister, P Liò, DJ Harrison, and O Arandjelović. Deep multiple instance learning with distance-aware self-attention, May 2023.

[87] KF Yeh, P Flood, W Redman, and P Liò. Learning linear embeddings for non-linear network dynamics with koopman message passing, May 2023.

[88] S Dittmer, M Roberts, J Gilbey, A Biguri, I Selby, A Breger, M Thorpe, JR Weir-McCall, E Gkrania-Klotsas, A Korhonen, E Jefferson, G Langs, G Yang, H Prosch, J Stanczuk, J Tang, J Babar, L Escudero Sánchez, P Teare, M Patel, M Wassin, M Holzer, N Walton, P Lió, T Shadbahr, E Sala, J Preller, JHF Rudd, JAD Aston, and CB Schönlieb. Navigating the development challenges in creating complex data systems. *Nature Machine Intelligence*, 5(7):681–686, Jul 2023.

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[90] J Yang, X-X Li, F Liu, D Nie, P Lio, H Qi, and D Shen. Fast multi-contrast mri acquisition by optimal sampling of information complementary to pre-acquired mri contrast. *IEEE Trans Med Imaging*, 42(5):1363–1373, May 2023.

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[92] X Lu, X Zhang, and P Lio. Gat-dns: Dns multivariate time series prediction model based on graph attention network. In *ACM Web Conference 2023 - Companion of the World Wide Web Conference, WWW 2023*, pages 127–131, Apr 2023.

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