List of Publications

The work carried out in this dissertation have appeared in the following peer-reviewed publications in reverse chronological order:

 T. Dash, S. Chitlangia, A. Ahuja, A. Srinivasan, "A review of some techniques for inclusion of domain-knowledge into deep neural networks", *Nature Scientific Reports*, 2022.

URL: https://doi.org/10.1038/s41598-021-04590-0

2. T. Dash, A. Srinivasan, L. Vig, A. Roy, "Using domain-knowledge to assist lead discovery in early-stage drug design", *International Conference on Inductive Logic Programming*, 2021.

URL: https://doi.org/10.1007/978-3-030-97454-1_6

3. T. Dash, A. Srinivasan, A. Baskar, "Inclusion of domain-knowledge into GNNs using mode-directed inverse entailment", *Machine Learning*, 2021.

URL: https://doi.org/10.1007/s10994-021-06090-8

4. T. Dash, A. Srinivasan, L. Vig, "Incorporating symbolic domain knowledge into graph neural networks", *Machine Learning*, 2021.

URL: https://doi.org/10.1007/s10994-021-05966-z

5. T. Dash, A. Srinivasan, R.S. Joshi, A. Baskar, "Discrete stochastic search and its application to feature-selection for deep relational machines", *International Conference on Artificial Neural Networks*, 2019.

URL: https://doi.org/10.1007/978-3-030-30484-3_3

 T. Dash, A. Srinivasan, L. Vig, O.I. Orhobor, R.D. King, "Large-scale assessment of deep relational machines", *International Conference on Inductive Logic Program*ming, 2018.

URL: https://doi.org/10.1007/978-3-319-99960-9_2 (*Winner of the Best Student Paper Award)

The author was involved in several other publications during his PhD. These publications do not constitute any content of this dissertation, but each publication has served as a motivation for the problem investigated in this dissertation. A non-exhaustive list of peer-reviewed publications is provided below.

G. Chhablani, A. Sharma, H. Pandey, T. Dash, "Superpixel-based Knowledge Infusion in Deep Neural Networks for Image Classification", ACM Southeast Regional Conference, 2022.

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URL: https://doi.org/10.1145/3476883.3520216
(*Winner of the Best Short Paper Award)
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2. A. Sonwane, G. Shroff, L. Vig, A. Srinivasan, T. Dash, "Solving Visual Analogies Using Neural Algorithmic Reasoning", *AAAI Student Abstract and Poster Program*, 2022.

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URL: https://arxiv.org/abs/2111.10361
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3. I. Olier, O.I. Orhobor, T. Dash, A.M. Davis, L.N. Soldatova, J. Vanschoren, R.D. King, "Transformational machine learning: Learning how to learn from many related scientific problems", *Proceedings of the National Academy of Sciences of the U.S.A.*, 2021.

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URL: https://doi.org/10.1073/pnas.2108013118
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4. S. Chitlangia, A. Sonwane, T. Dash, L. Vig, A. Srinivasan, G. Shroff, "Using Program Synthesis and Inductive Logic Programming to solve Bongard Problems", *International Workshop on Approaches and Applications of Inductive Programming*, 2021.

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URL: https://lr2020.iit.demokritos.gr/online/IJCLR_2021_paper_21.pdf
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5. H. Shah, A. Vaswani, T. Dash, R. Hebbalaguppe, A. Srinivasan, "Empirical Study of Data-Free Iterative Knowledge Distillation", *International Conference on Artificial Neural Networks*, 2021.

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URL: https://doi.org/10.1007/978-3-030-86365-4_44
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6. S. Krishnan, R. Khincha, L. Vig, T. Dash, A. Srinivasan, "A Case Study of Transfer of Lesion-Knowledge", MICCAI Workshop on Medical Image Learning with Less Labels and Imperfect Data, 2020.

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URL: https://doi.org/10.1007/978-3-030-61166-8_15
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7. K. Mahajan, M. Sharma, L. Vig, R. Khincha, S. Krishnan, A. Niranjan, T. Dash, A. Srinivasan, G. Shroff, "CovidDiagnosis: Deep Diagnosis of Covid-19 Patients using Chest X-rays", *MICCAI Workshop on Thoracic Image Analysis*, 2020.

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URL: https://doi.org/10.1007/978-3-030-62469-9_6
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8. S. Yalburgi, T. Dash, R. Hebbalaguppe, S. Hegde, A. Srinivasan, "An Empirical Study of Iterative Knowledge Distillation for Neural Network Compression", European Symposium on Artificial Neural Networks, Computational Intelligence and Machine Learning, 2020.

URL: https://www.esann.org/.../proceedings/2020/ES2020-205.pdf

 T. Dash, S.N. Dambekodi, P.N. Reddy, A. Abraham, "Adversarial neural networks for playing hide-and-search board game Scotland Yard", Neural Computing and Applications, 2018.

URL: https://doi.org/10.1007/s00521-018-3701-0

 A. Saboo, A. Sharma, T. Dash, "GASOM: Genetic Algorithm Assisted Architecture Learning in Self Organizing Maps", International conference on Neural Information Processing, 2017.

URL: https://doi.org/10.1007/978-3-319-70087-8_25

11. P.P. Pai, T. Dash, S. Mondal, "Sequence-based discrimination of protein-RNA interacting residues using a probabilistic approach", *Journal of Theoretical Biology*, 2017.

URL: https://doi.org/10.1016/j.jtbi.2017.01.040

Brief Biography of the Candidate

Tirtharaj Dash started his PhD in Machine Learning in January 2017 in the Department of Computer Science and Information Systems at BITS Pilani, Goa Campus, under the supervision of Senior Professor Ashwin Srinivasan. He received a Master of Technology (M.Tech) degree in Computer Science and Engineering, with one year thesis, from VSSUT, Burla in the year 2014 and a Bachelor of Technology (B.Tech) degree in Information Technology from NIST Berhampur in the year 2012. He was the topper of his batch, both in his M.Tech. and B.Tech, and the university and institute awarded him the Silver Medals. In August 2015, Tirtharaj joined the Department of Computer Science and Information Systems at BITS Pilani, Goa Campus, as an Assistant Professor (Grade-II). In June 2020, he was inducted to the Anuradha and Prashanth Palakurthi Centre for Artificial Intelligence Research (APPCAIR), BITS Pilani, Goa Campus. Before joining BITS, he worked as an Assistant Professor in the School of Computer Science at NIST Berhampur for over a year, from 2014–2015. He also worked as an IASc-INSA-NASI Summer Research Fellow at ISI Kolkata in 2015. His research areas of interest are Deep Learning, Neuro-Symbolic Learning, Graph Representation Learning and Machine Learning. He is a regular member of the ACM.

Brief Biography of the Supervisor

Ashwin Srinivasan received his PhD from the School of Electrical Engineering and Computer Science at the University of New South Wales, Australia, in 1991. His dissertation examined the use of defeasible logic for the photo-interpretation of remotely sensed data and investigated the comparative advantage of this representation over methods like Multivariate Gaussian Analysis and Dempster Shafer Theory. During the latter half of 1990, he developed a non-monotonic logic-based system for interpreting chemical pathology data. This was awarded the Pacific Diagnostic's Prize and recommended for use in all hospitals in the state of New South Wales. In 1991, Ashwin joined the ILP group at the Turing Institute, Scotland and—with S. Muggleton (now at Imperial College, London) worked on the application of Algorithmic Information Theory to noise-detection and non-monotonic learning in ILP. From 1993, Ashwin was a member of the Oxford University Computing Laboratory, where he was involved in pioneering applications of ILP systems to difficult real-world problems in molecular biology and chemistry. From 1998– 2000 he was the Nuffield Trust Research Fellow in Medical Mathematics and a Research Fellow of Green College, Oxford. In 2001, he was appointed to a University Lecturership in Computation at Oxford and a Fellowship in Computation at St Peter's College. Prior to this, he has also been a member of Wolfson College, Oxford. In 2003, he moved to the IBM Research – India, as a Research Staff Member. In 2009, he was awarded a Ramanujan Fellowship by the Department of Science and Technology of the Government of India. In 2010, he took up the post of Professor at the newly formed South Asian University and became the founder Dean of the Faculty of Mathematics and Computer Science. He moved to the IIIT-D in Sept. 2012 and in Jan 2015 to BITS Pilani, Goa Campus. He was also a Visiting Professor at the Computing Laboratory, University of Oxford, and is a Visiting Professorial Fellow at the School of Computer Science and Engineering, University of New South Wales.

Brief Biography of the Co-supervisor

Sukanta Mondal works in the field of computational biology and bioinformatics to address various challenging questions in bio-molecular science. He received his PhD degree from Indian Institute of Science in 2007, under the supervision of Prof. Ramakumar S, for thesis work titled "Contributions to venominformatics: sequence-structure-function studies of toxins from marine cone snails. Application of order-statistics filters for detecting membrane-spanning helices". After his doctoral studies, Dr. Mondal moved to National Institutes of Biomedical Innovation, Health and Nutrition (NIBIOHN), Japan, for pursuing post-doctoral research on "Development of an international pharmaceutical innovation value chain for in silico drug discovery" under the supervision of Prof. Kenji Mizuguchi. Gathering rich experience at both national and international levels, he initiated his Annotate Biomolecules Computationally (ABC) group in the year 2012, which currently has various doctoral, graduate and undergraduate students working on protein functional annotation.