

# Mangal Prakash

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## PROFESSIONAL EXPERIENCE

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### Team Lead (ML Molecular Property Prediction)

Oxford, UK

*Exscientia*

Nov 2022 – Present

- Line managed cross-functional team of 4 AI research scientists and senior scientists to execute projects in small molecule property prediction domain.
- Led or collaborated on upto 4 concurrent projects in areas such as development of generative models for protein-ligand pose prediction, active learning for compound selection and development of predictive models for ligand property predictions.
- Spearheaded development of novel Deep Learning based algorithms for molecular representation learning.
- Conceptualized and launched projects with computational designers, medicinal chemists, research software engineers that may be important for company's future value proposition.
- Led the efforts for hiring of research scientists and interns.
- Supervised an intern on a research project for development of novel clinical image segmentation algorithms (paper in preparation).

### AI Research Scientist

Oxford, UK

*Exscientia*

Aug 2021 – Present

- Created an extensive benchmark to assess traditional and ML-based docking algorithms for self-docking.
- Developed diffusion model based small molecule docking algorithms for fast and accurate ML-based pose prediction.
- Improved the in-house clinical imaging platform by building novel and scalable supervised and unsupervised Deep Learning based image restoration models to increase image analysis throughput.
- Conceptualized and executed a project to ingest and learn from multiple clinical data modalities including molecular graphs and microscopy images for patient stratification and *in-silico* drug screening.

## EDUCATION

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### Max-Planck Institute (CBG)/ Technische Universität Dresden

Dresden, Germany

*PhD in Computer Science — Summa Cum Laude*

Aug 2017 – July 2021

### University of Minnesota, Twin Cities

Minneapolis, USA

*MS in Electrical Engineering*

Aug 2014 – Dec 2016

### National Institute of Technology, Durgapur

Durgapur, India

*B.Tech in Electrical Engineering*

Aug 2010 – April 2014

## SELECTED ACADEMIC PROJECTS

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### Unsupervised deep image restoration | *PyTorch, Generative models, Deep Learning* Aug 2019 – July 2021

- Developed a novel state-of-the-art approach to model unsupervised diversity denoising and artefact removal tasks within variational autoencoder framework using learned/estimated model of imaging noise. Results published in ICLR 2021 and ICLR 2022.
- Introduced Gaussian Mixture Models based parametric representation of camera noise characteristics for training deep learning based algorithms for fully unsupervised denoising. Results published in IEEE ISBI 2020.

### Few shot cell and nuclei segmentation | *Python, TensorFlow, Deep Learning* Jan 2019 – June 2020

- Analyzed the impact of deep learning based unsupervised denoising for cell segmentation in presence of limited ground truth annotations. Results published in IEEE ISBI 2020.
- Implemented end-to-end training schemes for joint unsupervised denoising and segmentation with very limited amount of segmentation ground truth available. Results published in BIC@ECCV 2020.

### Consensus segmentation | *Python, Java, PyTorch, ILP solvers* Aug 2018 – July 2021

- Created a framework for obtaining diverse plausible segmentation for objects of interest using only noisy input images. Results published in ICLR 2021.
- Working on an ILP based optimization formulation for segmentation fusion from different segmentation sources using active learning based framework.

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## SELECTED PUBLICATIONS (*google scholar citations: 429, h-index: 11, i-10 index: 13*)

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- M. Prakash**, M. Delbracio, P. Milanfar, and F. Jug. *Interpretable Unsupervised Diversity Denoising and Artefact Removal*. International Conference on Learning Representations (ICLR) 2022 (**Selected for Spotlight presentation**).
- M. Prakash**, A. Krull, and F. Jug. *Fully Unsupervised Diversity Denoising with Convolutional Variational Autoencoders*. International Conference on Learning Representations (ICLR) 2021.
- S. Haller, **M. Prakash**, L. Hutschenreiter, T. Pietzsch, C. Rother, F. Jug, P. Swoboda, and B. Savchynskyy. *A Primal-Dual Solver for Large-Scale Tracking-by-Assignment*. Proceedings of the 24th International Conference on Artificial Intelligence and Statistics (AISTATS) 2020.
- M. Prakash**, T-O. Buchholz, D. Schmidt, A. Krull, and F. Jug. *DenoiSeg: Joint Denoising and Segmentation*. Bio Image Computing Workshop@ECCV 2020 (**Selected for oral presentation**).
- M. Prakash**, M. Lalit, P. Tomancak, A. Krull, and F. Jug. *Fully Unsupervised Probabilistic Noise2Void*. IEEE International Symposium on Biomedical Imaging (ISBI) 2020 (**Selected for oral presentation**).
- M. Prakash**, T-O. Buchholz, M. Lalit, P. Tomancak, F. Jug, and A. Krull. *Leveraging Self-Supervised Denoising for Image Segmentation*. IEEE International Symposium on Biomedical Imaging (ISBI) 2020.
- A. Krull, T. Vicar, **M. Prakash**, M. Lalit, and F. Jug. *Probabilistic Noise2Void: Unsupervised Content-Aware Denoising*. Frontiers in Computer Science, 2020.
- A. Jain, V. Ulman, A. Mukherjee, **M. Prakash**, M.B. Cuenca, L.G. Pimpale, S. Münster, R. Haase, K.A. Panfilio, F. Jug, S.W. Grill, P. Tomancak, and A. Pavlopoulos. *Regionalized tissue fluidization is required for epithelial gap closure during insect gastrulation*. Nature Communications, 2020.
- H. Vignes, C. Vagena-Pantoula, **M. Prakash**, C. Norden, F. Jug, and J. Vermot. *Extracellular Mechanical Forces Drive Endocardial Cell Volume Decrease During Cardiacvalve Morphogenesis*. Developmental Cell, 2021.
- M. Slabodnick, S. Tintori, **M. Prakash**, C. Higgins, A. Chen, T. Cupp, T. Wong, E. Bowie, F. Jug, B. Goldstein. *Afadin and zyxin contribute to coupling between cell junctions and contractile actomyosin networks during apical constriction*. PLOS Genetics, 2023.
- D. Alves-Afonso, A. Ryan, A. Lahola-Chomiak, **M. Prakash**, F. Jug, C. Modes, and J. Tabler. *Collagen structure maintains mesenchymal stem cell fate and nuclear shape in embryonic sutures*. Under review at Cell Reports.

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## INVITED TALKS

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- Unsupervised Diversity Denoising and Artefact Removal with Generative Models** | *SIAM ISS2* Mar 2022
- Fully Unsupervised Diversity Denoising with Variational Autoencoders** | *MDC Berlin* June 2021
- Leveraging Self-Supervised Denoising for Image Segmentation** | *QBI, University of Oxford* Jan 2021

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## ACADEMIC COMMUNITY INVOLVEMENT

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- Reviewer for **ICML 2023, NeurIPS 2022, ICLR 2022, NeurIPS 2021, ISBI 2021**
- Teaching Assistant for different courses in graduate school and mentor for Deep Learning and image processing hackathons

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## SCHOLARSHIPS AND AWARDS

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- College of Science and Engineering Fellowship** | *University of Minnesota for graduate studies* 2014-2015
- Graduate Research and Teaching Assistantship** | *University of Minnesota for graduate studies* 2015-2016
- Summer Research Fellowship** | *Awarded by Indian Academy of Sciences but could not undergo internship* 2013
- Merit certificate** | *Awarded by CBSE to top 0.1% students nationwide for matriculation exams* 2007

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## PROFICIENT TECHNICAL SKILLS

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- Programming Languages:** Python (advanced), Java (advanced), MATLAB (basic)
- Deep Learning Frameworks:** PyTorch (advanced), Keras (good), TensorFlow (good)
- Developer Tools:** Git (advanced), Github (advanced), PyCharm (advanced), Eclipse (advanced)
- Bioimage Analysis Softwares:** Fiji/ImageJ (advanced), Ilastik (advanced), Labkit (advanced)
- Others:** Light sheet microscopy (basic), Latex (advanced)