Ankit Agrawal

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Career Objective
I seek a career in teaching and interdisciplinary research in life sciences, computational biology, biophysics, and artificial intelligence.

Research Goal
I want to keep the mainstream focus on computational biology. Still, I wish to be closely involved with experimental biologists so that our combined research effort has a more significant impact on society.

Job Profile
- Postdoctoral researcher in computational single-cell biology in Dominic Grün lab since July 2021 at Lehrstuhl für Computational Biology of Spatial Biomedical Systems, University of Würzburg, Würzburg, Germany
- Postdoctoral researcher in computational single-cell biology in Dominic Grün lab from Jan 2021 - June 2021 at Max Planck Institute of Immunobiology and Epigenetics, Freiburg im Breisgau, Germany
- Postdoctoral fellow in bone tissue data analysis in Elazar Zelzer lab from Nov 2018 - Dec 2020, at Department of Molecular Genetics, Weizmann Institute of Sciences, Rehovot, Israel

Education Profile
- Ph.D. in 'Computational Biology' (awarded on October, 2019) from "The Institute of Mathematical Sciences (IMSc), Chennai" affiliated to Homi Bhabha National Institute (HBNI), Mumbai, India
- M.Tech. (2012) in Bioinformatics from IIIT Hyderabad, Hyderabad, India
- M.Sc. (2010) in Bioinformatics from The University of Allahabad, Allahabad, India
- B.Sc. (2008) in Applied Science from The University of Allahabad, Allahabad India
- Intermediate (2005) from Board of High School and Intermediate Education, UP India
- High School (2003) from Board of High School and Intermediate Education, UP India

Thesis Title
Nuclear Architecture from Chromosomes to Motifs (ResearchGate DOI:10.13140/RG.2.2.22726.32327)

Thesis supervisor
Gautam I. Menon (IMSc) (Advisor)
Rahul Siddharthan (IMSc) (Co-advisor)

Google scholar profile
Ankit Agrawal https://scholar.google.com/citations?hl=en&user=ey8X7BwAAAAJ

Github profile
@nkit https://github.com/ankitbioinfo

ResearchGate profile R^G
Ankit Agrawal https://www.researchgate.net/profile/Ankit_Agrawal9

Journal Publications

- **Ankit Agrawal**, Dominic Grün "Prediction of cell-cell communication across cell types in the multimodal integration of spatially resolved transcriptomics and single-cell RNA-seq data" (under preparation)
- Sarah Rubin, Anne Seewald, Tomer Stern, Paul Villoutreix, Adrian Baule, **Ankit Agrawal**, Elazar Zelzer "Self-organization of the chondrocytes clones in embryonic growth plate tissue reveals no 3D stacking of cells in a column-like structure; instead, they formed random clusters" (under preparation and I am also one of the corresponding author)
- S. Rubin, **A. Agrawal**, J. Stegmaier, S. Krief, N. Felsenthal, J. Svorai, Y. Addadi, P. Villoutreix, T. Stern, E. Zelzer "Application of 3D MAPs pipeline identifies the morphological sequence chondrocytes undergo and the regulatory role of GDF5 in this process" Nature Communications (2021)
- **A. Agrawal**, N. Ganai, S. Sengupta and G. I. Menon "Nonequilibrium Biophysical Processes Influence the Large-Scale Architecture of the Cell Nucleus" Biophysical Journal (2019)
- **A. Agrawal**, S. V. Sambare, L. Narlikar and R. Siddharthan "THiCweed: fast, sensitive motif finding by clustering big data sets" Nucleic Acids Research (2018) 46(5), e29
- **A. Agrawal**, N. Ganai, S. Sengupta and G. I. Menon "Chromatin as active matter" Journal of Statistical Mechanics: Theory and Experiment (2017) 014001
- **A. Agrawal**, C. Sarkar, S. K. Dwivedi, N. Dhasmana and S. Jalan "Quantifying randomness in protein-protein interaction networks of different species: A random matrix approach" Physica A: Statistical Mechanics and its Applications (2014) 404, 359-367

Abstract Publications

- A. Agrawal, N. Ganai, S. Sengupta and G. I. Menon "A First-principles Approach to Large-scale Nuclear Architecture" Biophysical Journal (2018) 114 (3), 444a-445a

Research Skills

- Single-cell analysis task and packages: Clustering (Leiden, Louvain), UMAP and TSNE representation, cell-type annotation, Python (Scanpy), R (RaceID, Scran, scater, scRNAseq, batchelor etc)
- Spatial-transcriptomics: Designing of RNA probes for seqfish+ protocol, detection of RNA spots using starfish pipeline for barcoding rounds of image-based transcriptome
- Image analysis task: Basic image registration and segmentation task
- Machine Learning and data science packages: Scikit-learn, PyTorch (beginner), Jupyter lab, MatplotLib, NetworkX, pandas, numpy, scipy, seaborn, hypothesis test etc
- Image Processing Packages: ImageJ, Ilastik, scikit-image, MATLAB
- Programming and scripting language: Moderate level (C, C++, and R); advance level (Python, LaTeX, and MATLAB)
- Simulation Software: LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator)
- Sequencing Software: NGS/Bioinformatics related tools (bedtools, deeptools, meme etc.)
- Visualization Software: VMD, Povray, MATLAB, Basic Blender
- HPC: Handling of Dockerfile installation in Linux like platform, Little experience with virtual machine and Kubernetes architecture

Dream Challenge Participation and Publications

- Rahul Siddharthan (IMSc), Leelavati Narlikar (NCL Pune), and I (IMSc) as a team participated in "ENCODE-DREAM in vivo Transcription Factor Binding Site Prediction 2016" challenge to take the task of predicting genome-wide in vivo binding of TFs in the given cell types. We built a classifier based on a machine learning model that predicts whether TF bounds a given region or not. Our team scored 10th rank out of total 33 participants.

- I also participated in the "Dream Idea Challenge Consortium 2016", where the task was to propose an idea to perform an experiment based on the concept of a 'data-driven model' rather than 'model-driven data.' My idea got carried forward to the first round. Later, organizers published a paper *"The inconvenience of data of convenience: computational research beyond post-mortem analyses"* Nature Methods Vol. 14, No. 10, 2017 and put all the participants' names under "DREAM Idea Challenge Consortium".

Invited Speaker

- Invited talk on "A Large Scale Model of Nuclear Architecture" at discussion meeting of "Aspects of gene and cellular regulation" held on August 2016, at *IMSc Chennai*, India
- Invited talk on "A Large Scale Model of Nuclear Architecture" at 3rd BSSE Annual Research Symposium" on Computational Bioengineering held on January 2017, at *IISc Bangalore*, India
- I gave a talk on " Nuclear Architecture from Chromosomes to Motifs" at Bar-Ilan University, Israel on 27 June, 2018
- I gave a talk on " Nuclear Architecture from Chromosomes to Motifs" at Weizmann institute of science, Israel on 28 June, 2018
- I gave a talk on " Nuclear Architecture from Chromosomes to Motifs" at Tel Aviv University, Israel on 3rd July, 2018
- I gave a talk on " Nuclear Architecture from Chromosomes to Motifs" at Technion - Israel Institute of Technology, Israel on 4th July, 2018

Conferences and Workshops

- Poster presentation in "TAU-ESPCI international summer school on self-organization and self-assembly: from physics and chemistry to biology" held in *Tel Aviv University*, Israel from September 8-12, 2019
- Attended "Methods and Problems in BioImaging Workshop" in *Weizmann Institute of Science*, Israel on June 24th, 2019
- Gave a talk on 'Higher-order Chromatin Architecture' in "Computaional Biology Annual Meeting" on March 22, 2018 at *IMSc*, Chennai
- Posters presentation in EMBO meeting "The nucleosome: From atoms to genomes" from August 30 to September 1, 2017, in *EMBL Heidelberg*, Germany
- Poster presentation in discussion meeting on "Emergence and Evolution of Biological Complexity" was organized at *NCBS Bangalore*, India from February 4-6, 2017
- Attended "The Interface of Biology and Theoretical Computer Science" meeting which held on December 19-21, 2016, at *NCBS Bangalore*, India
- Poster presentation in discussion meeting on "Conflict & Cooperation in Cellular Populations (CCCP)" was organized at *NCBS Bangalore*, India from October 16-19, 2016
- Poster presentation in discussion meeting on "Mechanical Forces in Cell Biology Information at the Cell & Tissue Scale" was organized at *NCBS Bangalore*, India from October 4-6, 2016
- Poster presentation in ICTS-ICTP program "Winter School on Quantitative Systems Biology" which held on December 2015, at *ICTS Bangalore*, India
- Attended "Advanced Workshop on Interdisciplinary View on Chromosome Structure and Function" which held on September 2014, at *ICTP, Trieste* Italy
- Attended "NCNSD (National Conference on Nonlinear Systems and Dynamics)" which held on July 2012, at *IISER Pune*, India
- Participated in the interaction session of "Science Conclave: A Congregation of Nobel Prize Winners" organized by *IIIT, Allahabad*, India in December 2009

Achievement

- Ph.D. fellowship provided by Government of India "Department of Atomic Energy"
- Achieved 10th all India rank in "Bioinformatics National Certificate Exam" (BINC-2013) conducted by JNU, DBT India
- Got EMBO Travel grant for attending the conference "The nucleosome: From atoms to genomes" from August 30 to September 1, 2017, in *EMBL Heidelberg*, Germany
- Got half funding for attending the workshop "Advanced Workshop on Interdisciplinary View on Chromosome Structure and Function" which held on September 2014, at *ICTP, Trieste* Italy

Coursera, edX certificates

- Accomplishment certificate of "Introduction to Artificial Intelligence" offered by Sebastian Thrun and Peter Norvig, passed with a score of 67.7%
- Accomplishment certificate of "Synapses, Neurons and Brains" offered by The Hebrew University of Jerusalem through coursera, with a score of 87.0%
- Accomplishment certificate of "Programmed cell death" offered by LMU through coursera, with a score of 52.8%
- Accomplishment certificate of "Case study: ChIP-seq data analysis" offered by HarvardX through edX, with a score of 71%

Details of Unpublished Ongoing Projects

1. Project Title: Prediction of cell-cell communication across cell types in the multimodal integration of spatially resolved transcriptomics and single-cell RNA-seq data

   Summary: Since the last decades, RNA-sequencing technologies have improved significantly from measuring bulk RNA-Seq to single-cell RNA-seq (scRNA-seq) to spatially-resolved transcriptomics (SRT). In scRNA-seq, we lose the information of spatial organization of tissue to achieve the whole transcriptome. At the same time, SRT provides an unprecedented opportunity to explore the architecture of tissue with a handful number of genes while preserving the spatial distribution of cells. Studies show that stem cells respond to the global environment by sensing the local niche microenvironment in which they communicate with surrounding cellular and non-cellular elements. The niche's microenvironment often consists of specialized and differentiated cells that interact physically or non-physically, secreting cell regulatory factors and maintaining the stem cell population. SRT is important for tissue homeostasis, development, and injury repair studies that are maintained through hardwired networks of stem cell communication and their environment.

   Cell-cell communication event refers to an interaction between secreted ligands and membrane receptors. These interactions can be physical (juxtacrine), intracellular (autocrine), or through diffusion (paracrine). We asked whether cell-cell communication is the source of the variation in the tissue or the presence of variation in the tissue niche responsible for cell-cell communication. First, we build a regression-based machine learning model to predict the cell type interaction rules from the niche neighborhood. Second, the communication of ligand-receptor genes and possible downstream target pathways inference using statistical hypothesis tests and regression models on top of the known cell-cell interactions. SRT data alone hindered understanding of cell heterogeneity, so the data integration of SRT and single-cell is the right approach to explore the full heterogeneity, tissue homeostasis, and cell-cell communication events.

2. Project Title: Self-organization of the chondrocytes clones in embryonic growth plate tissue reveals no 3D stacking of cells in a column-like structure; instead, they formed random clusters

   Summary: The growth plate is a highly organized tissue responsible for postnatal long bone growth. H&E 2d staining reveals that the column-like arrangement of chondrocytes in the growth plate is an essential factor of bone elongation but hitherto no clear understanding of how long columns formes. We performed clonality cell tracing experiments on confetti mice at ages E18.5 and P40. In the embryonic growth plate of tibia and fibula bones, stochastic sparse labeling of clonal chondrocytes through 3d image analysis reveals that proliferated chondrocytes grow in self-assembled random small clusters consisting of 3-30 cells. The volume distribution of growing cell clusters follows the K-gamma distribution theory given by Aste and Di Matteo [PRE 2008]. It means that volumes are distributed at random, so the positions of the cells also.

This result is a paradigm shift in the fundamental concept of bone growth in the musculoskeletal developmental biologist community. I also compared the clonal labeled cell growth clusters (real) with nonclonal nonlabelled cell growth clusters (random) along the proximal-distal bone growth axis. We found no significant differences in the spatial profiles of gyration (Rg) radius, global and local orientational order parameters, volume, surface area, asphericity index, average degree, and volume fraction. This finding lets us ask more questions about the mechanism of chondrocyte cells division and maintaining the density and different shapes along three (resting, proliferative and hypertrophic) zones. To find precisely the cluster formation process is the task of future research.

Teaching Plan

I am interested in teaching graduate-level courses in bioinformatics, systems biology, biophysics, and statistics. But I can also prepare a few additional topics from machine learning, biological tissue image analysis, and materials related to single-cell multi-modal analysis on-demand for research-oriented students.