Arindam Paul

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Information Apartment 3W E-mail: arindam.paul@eecs.northwestern.edu

Evanston, IL 60208 USA Website: www.arindampaul.me

Interests Machine Learning, Deep Learning, Natural Language Processing, Materials Informatics, Cheminformatics

PROGRAMMING Programming: Python, MATLAB, R

Skills Data Science: Keras, Tensorflow, PySpark, Scikit-Learn, XGBoost, RDKit, Gensim, NLTK, Pandas, Numpy,

Seaborn, Matplotlib, Theano, PyTorch

Web Development: HTML/Markdown, CSS, JavaScript, Ruby On Rails

Education Northwestern University, Evanston, Illinois

Ph.D. Candidate, Computer Science (Expected graduation date: Jul 2019.)

Advisors: Prof. Alok Choudhary, Prof. Ankit Agrawal

Northwestern University, Evanston, Illinois

Master of Science, Computer Science, Summer 2014

Birla Institute of Technology & Science, Pilani, Rajasthan India

Master of Engineering (Hons.), Software Systems, May 2012

• Dissertation: Designing an efficient Distributed Computing Solution for Data Mining

Birla Institute of Technology & Science, Pilani, Rajasthan India

Bachelor of Engineering (Hons.), Chemical Engineering, Dec 2009

• Thesis: Detecting Sybil Attacks in P2P networks using Psychometric Analysis

RESEARCH EXPERIENCE Northwestern University, Evanston, Illinois USA

Research Assistant Fall '12 - present

Ensemble Nets on Mixed Representations for Chemical Property Prediction (Tensorflow, Keras) Sep '18 -

- Created CheMixNet a deep neural network that combines molecular fingerprints to develop a generalized architecture for chemical property prediction
- Designed SINet a deep network that combines two different textual representations SMILES and InChI for predicting chemical properties
- Expanded SINet for transfer learning tasks from a 2.3 million dataset to a smaller 350 compound dataset
- Developed ChemsembleNet a deep network that combines different textual, molecular fingerprints and molecular graph representations of molecules to achieve better results than individual representations

Deep Learning-based Predictive Model for Additive Manufacturing (Tensorflow, Keras) Nov '16 -

- Created Hidden Markov models for time series analysis of heat flux data
- Investigating Recurrent Neural Network models to predict point-wise temperature information for accelerating additive manufacturing simulations

Solar Cell Efficiency Prediction using Molecular Fingerprints (Tensorflow, Scikit Learn) Mar '16 -

- \bullet Designed Deep Neural Network and Random Forest models for predicting power conversion efficiency of solar cells using chemical fingerprints, and achieved mean square percentage error between 1.5-2 %
- Designed an online application for material scientists to get an estimation of power efficiency

Very Deep Neural Networks for Predicting Formation Stability (Tensorflow) Mar '16 - Sept '17

- Constructed Neural Network Models with 18-25 layers to predict formation energy of a chemical compound
- Attained 20 % higher accuracy than the state-of-the-art models using Random Forests that would allow
 domain scientists to explore millions of possible compounds

Ensemble Learning-based Guided Optimization for Aircraft Design (MATLAB, Python) Oct '15 - Dec '17

- Created intelligent sampling algorithms to explore the constrained search space for candidate microstructures
- Developed Feature Ranking-based Technique for Search Space Reduction of Constrained Non-Convex Optimization
- Achieved 100x candidate microstructures compared to state-of-the-art methods that can accelerate the design-to-experiment life-cycle

Convolutional Neural Nets for Thematic Image Classification in Pinterest(Torch)

- Harnessed Association Rule Mining for thematic label curation
- Developed ConvNet Models for hierarchical classification that led to automated image categorization based on themes

Classification of Anonymous Posts using Recurrent Neural Networks (Tensorflow) Jan '15 - May '16

- Generated vectorizer models using Word2vec trained on crowd-sourced (Urban Dictionary) & psycholingual (LIWC) dictionaries (Gensim)
- Attained prediction accuracy of 79.8 % and 78.1 % using LSTMs and ensemble models respectively

Facebook Confessions & Yik Yak

Jun '14- Dec '14

Oct '15 - Sep '16

- Studied question asking about sensitive topics in anonymous forums
- Designed a system to automatically identify and classify taboo posts in anonymous forums with good accuracy

Learning from Ads:Reverse-engineering demographics and interests

Feb '13-May '14

- Created synthetic user profiles with different demographic and interest features and collecting ad traffic
- Created a model by using cross-validation which can predict user features from resulting data-set and ground-truth
- Application of the model to cellular web-data to predict user's demographics and interests on-the-fly

 $Graduate\ Researcher$

Spring '10 - Spring '12

Designing an efficient Distributed Computing Solution for Data Mining

Fall '11 -Spring '12

- Created a Beowulf Linux(Ubuntu) cluster using OpenMPI library project
- Implemented parallel implementation of K-means for OpenMPI
- Bench-marked sequential and parallel OpenMPI implementations of K-means clustering algorithm
- Compared the performance with the control Hadoop cluster

Preventing Sybil attacks in P2P systems using Psychometric Tests $\,$

Fall '09 - Spring '11

- Suggested a novel approach to use Psychometric Tests (Luscher Color Test and Myers Briggs Type Indicator Test) to evaluate psychometric index of users
- Cluster nodes with similar scores and in case of a particularly high-frequency zone, we treat these nodes as suspicious and further use CAPTCHAs to remove false positives.

Software Quality Evaluation using Fuzzy Multi-Criteria Approach

Spring '10- Spring '11

- Employed fuzzy ratings and weights to software attributes and proposed a comprehensive model for calculating overall software quality based on ISO/IEC 9126 model.
- Tested on multiple university softwares and one industrial application.

TEACHING EXPERIENCE

Northwestern University, Evanston, Illinois USA

Teaching Assistant

Winter '14 -

Assisted the instructor in teaching the following undergraduate level courses. Duties included sharing of responsibilities for lectures, exams, homework assignments, grades, office hours and leading computer lab

- EECS 510 Social Media Mining, Spring '17, '18 & '19
- EECS 214 Data Structures and Data Management, Fall 2015

• EECS 110 Introduction to Computer Programming (Python), Winter & Spring 2014, Winter 2015

Guest Lecturer Spring '16

EECS 510 Social Media Mining

- Impact of "likes" and "reactions" on social media
- Anonymity in Social Media
- Crawling and scraping the web

Instructor Summer '16

MGLC Transferable Skills Workshop on Machine Learning

Attended by McCormick Graduate students and faculty

- What and Why of Machine Learning?
- Algorithms
- Application
- Introduction to Deep Learning

BITS Pilani, Rajasthan, India

Teaching Assistant Jan - May '12

Assisted the instructor in teaching the following undergraduate level courses. Duties included sharing of responsibilities for exams, homework assignments, grades and leading computer lab exercises.

• CS/IS 332 Introduction to Database Systems and Application, Spring 2012.

Publications: Journals

- A. Paul, A. Furmanchuk, W. Liao, A. Choudhary and A. Agrawal. "Organic Molecule Prediction for Photovoltaic Applications Using Extremely Randomized Trees", Journal of Molecular Informatics (accepted)
- A. Paul, W. Liao, A. Choudhary and A. Agrawal. "Mining Anonymous Taboo Confessions using Psycho-lingual and Crowd-Sourced Dictionaries for Emotional Wellbeing", *Journal of Health Informatics Research (under review)*
- A. Paul, W. Liao, A. Choudhary and A. Agrawal. "Text Translation as Data Augmentation for Neural Network Modeling of Mental Health Confessions", Journal of Public Library of Science (PLOS One) (in preparation)
- A. Paul, W. Liao, A. Choudhary and A. Agrawal. "ChemsembleNet: A generalizable, transferable architecture for predicting chemical properties using multiple representations", *Journal of Computational Chemistry (in preparation)*
- A. Paul, P. Acar, W. Liao, A. Choudhary, V.Sundararaghavan and A. Agrawal. "Microstructure Optimization with Constrained Design Objectives using Machine Learning-Based Feedback-Aware Data-Generation", *Journal of Computational Materials Science*, Apr 2019
- D.Jha, L.Ward, A. Paul, W. Liao, A. Agrawal, A. Choudhary and C. Wolverton. "ElemNet: Deep Learning the Chemistry of Materials From Only Elemental Composition", Nature Scientific Reports, Nov 2018
- M.Mozaffar, A. Paul, R. Al-Bahrani, S. Wolff, A. Choudhary, A. Agrawal, K. Ehmann and J.Cao. "Data-Driven Prediction of the High-Dimensional Thermal History in Directed Energy Deposition Processes via Recurrent Neural Networks", Manufacturing Letters, Sep 2018
- A. Paul, P. Acar, R.Liu, W. Liao, A. Choudhary, V. Sundararaghavan and A. Agrawal. "Data Sampling Schemes for Microstructure Design with Vibrational Tuning Constraints", *Journal of American Institute of Aeronautics and Astronautics*, Mar 2018
- K Haribabu, C.Hota and A. Paul "GAUR: A Method to Detect Sybil Groups in Peer-to-Peer Overlays", International Journal of Grid and Utility Computing, 2012 Vol.3 ISSN: 1741-847X

http://dx.doi.org/10.1504/IJGUC.2012.0477655

J.S. Challa, A.Paul*, Y.Dada, V.Nerella, P.R. Srivastava and A.P.Singh "Integrated Software Quality Evaluation: A Fuzzy Multi-Criteria Approach", Journal of Information Processing Systems (JIPS): Korean Information Processing Society, Volume 7, Number 3 (September 2011) ISSN: 1976-913X. http://dx.doi.org/10.3745/JIPS.2011.7.3.473

* = co-first author

Publications: Conferences

A. Paul, D.Jha, W. Liao, A. Choudhary and A. Agrawal. "Transfer Learning Using Ensemble Neural Nets for Organic Solar Cell Screening", International Joint Conference on Neural Networks, 2019

Z.Yang, D. Jha, A. Paul, W. Liao, A. Choudhary and A. Agrawal. "Generative adversarial networks with mixture density networks for inverse modeling in materials microstructural design", 28th ACM Conference on Information and Knowledge Management (CIKM) (under review)

A. Paul, M. Mozaffar, Z. Yang, W. Liao, A. Choudhary, J.Cao and A. Agrawal. "A real-time iterative approach for temperature profile prediction in additive manufacturing processes", 6th IEEE International Conference on Data Science and Advanced Analytics (DSAA), 2019 (in submission)

A. Paul, D.Jha, R. Al-Bahrani, W. Liao, A. Choudhary and A. Agrawal. "CheMixNet: Mixed DNN Architectures for Predicting Chemical Properties using Multiple Molecular Representations", NIPS Workshop on Machine Learning for Molecules and Materials, 2018

R. Liu, D. Palsetia, A. Paul, R. Al-Bahrani, D. Jha, W. Liao, A. Agrawal, and A. Choudhary. "PinterNet: A Thematic Label Curation Tool for Large Image Datasets", Proceedings of the Workshop on Open Science in Big Data at IEEE Bigdata Conference, 2016.

A. Paul, A. Agrawal, W. Liao, and A. Choudhary. "AnonyMine: Mining anonymous social media posts using psycho-lingual and crowd-sourced dictionaries", Proceedings of the Workshop on Issues of Sentiment Discovery and Opinion Mining at 22nd Annual ACM Conference on Knowledge Discovery and Data Mining, 2016.

J.Birnholtz, N.A.R. Merola, and A. Paul. "Is it Weird to Still Be a Virgin?:? Anonymous, Locally Targeted Questions on Facebook Confession Boards", Proceedings of the 33rd Annual ACM Conference on Human Factors in Computing Systems. ACM, 2015.

A. Paul, Varuni G., J.S. Challa, and Y. Sharma "HADCLEAN: A Hybrid Approach for Data Cleaning Techniques in Data Warehouses", Proceedings of the IEEE International Conference on Information Retrieval and Knowledge Management (CAMP), Kuala Lumpur, March, 2012

J.S. Challa, A.Paul*, Y. Dada, V. Nerella, and P.R. Srivastava "Quantification of Software Quality Parameters using Fuzzy Multi-Criteria Approach," Proceedings of the IEEE International Conference on Process Automation Control and Computing (PACC) 2011, Combatore, July, 2011

K Haribabu, A.Paul*, and C. Hota "Detecting Sybils in Peer-to-Peer Overlays using Psychometric Analysis Methods,", Proceedings of the 25th IEEE International Conference on Advanced Information Networking and Applications (AINA), Singapore, March 2011

Professional Experience

Northwestern Mutual Life Insurance, Milwaukee, Wisconsin

Machine Learning Intern

Jun '18 - Aug '18

- Developed distributed image to text conversion algorithms for detecting responses from scanned question-
- Designed a noise reduction algorithm to denoise scanned and photocopied questionnaires

EDT, New York City, New York

Data Science Consultant

Nov '16 -

- Provided subject matter expertise to develop algorithms for topic mining on legal documents
- \bullet Assisted in designing models for profanity detection from company-wide email database

Narus Inc. - A Boeing Company, Sunnyvale, California

Summer Research Intern Jun '13 - Sep '13

- Understanding Collaboration Among Online Advertising and Analytics Services
- Observed multiple 3rd-party services sharing user's information with each other
- Investigated how these services use means to obfuscate parameter sharing

Awards & Honors

- McCormick Dean's Commendation Fellowship, during 6th year of PhD (2017-2018)
- Predictive Science and Engineering Design Fellowship, during 5th year of PhD (2016-2017)
- Segal Design Cluster Fellowship, during 3rd year of PhD (2014-2015)
- Walter P. Murphy Fellowship, during 1st year of PhD (2012-2013)
- BITS Pilani Merit-cum-Need Scholarship during undergraduate study
- Among 10 doctoral students across Northwestern selected for summer-long Research Communication Workshop, 2016
- Best TA award for recognition of teaching excellency as Teaching Assistant for Database Systems and Applications (BITS Pilani 2012)
- All India Rank 1 in BITS HDSAT (admission test for graduate programs at BITS Pilani) in Software
- All India Rank 64 & State Rank 9 in National Science Olympiad among more than half million participants during freshmen year of high-school

LEADERSHIP

- President and Treasurer , Northwestern Toastmasters Club (2015-16, 2016-17)
- President and Founding Member, Northwestern Creative Writing Club
- President, Northwestern University Cricket Club
- Co-Facilitator, Northwestern Dialogue Group
- Mentor, Brave Initiatives (http://www.braveinitiatives.com/)

Side Projects

- Selected Course & Developed a Sentiment Analysis Tool to find the most interesting or controversial events at the 2014 Golden Globe Awards from user-Tweets (Python) Spring '14
 - Developed a web application to track a portfolio of a user's stocks. Used data mining techniques to analyze and predict stock and portfolio performance using historical data. (Perl, SQL)
 - Developed a real-time tool starts an alarm when a designated bus is 'x' (customizable) min away from the closest bus stop by scraping CTA bus tracker webpage (Python). Fall '14.